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Machine learning-based State-of-Health estimation of Lithium-Ion batteries from narrow voltage intervals

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Accurate estimation of lithium-ion battery state of health (SOH) is essential for safe and efficient operation; however, many existing methods require long measurement periods or full charge–discharge cycles, limiting their practical applicability. This work presents a fast data-driven SOH evaluation approach based on a narrow voltage interval measured during a fully controlled charging phase. The method enables reliable SOH assessment using only a short segment of the voltage curve, allowing frequent evaluation during normal battery operation. The approach is validated using eight open datasets from Aalto University and the Joint Research Centre (JRC), covering four different current rates and four temperature values, and spanning the full range of battery aging from a brand-new state to end-of-life. An optimal voltage interval is identified based on its strongest correlation with SOH across the widest possible range of charging protocols and ambient conditions. The corresponding voltage curve is then used for model-based SOH estimation. A data-driven model is developed to capture the relationship between the measured voltage curve and SOH. A long short-term memory (LSTM) neural network is selected due to its ability to handle short time sequences of consecutive voltage curves. The proposed method achieves high accuracy across all tested conditions, with a worst-case RMSE below 1%. The results demonstrate that accurate SOH estimation can be achieved using only narrow voltage segments, making the method suitable for real-time implementation in battery management systems.

A Multi-Scale Framework for Holistic Prismatic Battery Thermal Management: Coupling Internal Dynamics with External Regulation

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Electrochemical heat generation in lithium-ion batteries is inherently non-uniform and strongly governed by internal states such as reaction current density and overpotential. Conventional battery thermal management systems rely on temperature-based control with uniform cooling, often leading to overdesign, excessive pumping power, and persistent thermal gradients. In this work, a spatially resolved electrochemical–thermal framework is developed by coupling a P2D model with a two-dimensional heat transfer model for prismatic cells. In addition, internal electrolyte channel geometries are incorporated to investigate their influence on coupled transport and heat generation behavior.

The model captures spatial and temporal heat generation and shows how electrolyte channels affect ion transport, reaction distribution, and temperature. Based on these electrochemical insights, an adaptive cooling strategy is proposed in which the local coolant flow rate is dynamically regulated as a function of spatial heat generation and temperature gradients. This approach enables targeted cooling in regions with high thermal activity while maintaining minimal baseline flow elsewhere. The cooling boundary condition is further linked to flow-dependent convective heat transfer, allowing realistic estimation of thermal response and pumping requirements.

The framework is evaluated under different channel configurations using key metrics including maximum temperature, temperature uniformity, and pumping power. Results demonstrate that electrolyte channel design improves transport uniformity and, when combined with adaptive cooling, significantly reduces peak temperature and intra-cell thermal gradients while lowering overall pumping power. The study highlights the potential of integrating electrochemical modeling with geometric design for thermal management of next-generation lithium-ion batteries.

A dual-head temporal convolutional network approach for cloud-based battery state-of-health prognostics in a digital twin

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Accurate State-of-Health (SoH) prediction is critical for reliable battery management systems (BMS) and their digital twins. Within the Horizon Europe project BATMAX, a cloud-based digital twin framework is being developed, integrating experimental and operational data with physics-based, data-driven, and hybrid models for advanced BMS. A central requirement is a data-driven SoH prognostic model achieving prediction errors well below a user-specified threshold of 3 % and suitable for cloud deployment.

This work presents a Temporal Convolutional Network (TCN) with a dual-head output architecture for capacity-based SoH estimation of lithium nickel manganese cobalt oxide (NMC) batteries. Training and validation utilize cycling datasets from multiple cycling test sites, covering diverse state-of-charge windows and a representative maritime load profile. The TCN's hyperparameters are adjusted via Bayesian optimization. The dual-head design features feed two parallel output heads: one predicts absolute SoH, the other predicts the incremental SoH degradation (ΔSoH). A composite loss function balances absolute accuracy with degradation-trend consistency, emphasizing the absolute SoH head and using the ΔSoH head as an implicit regularizer.

Testing on held-out data subsets across different SoC windows yields root-mean-square and maximum absolute errors of 1 %. This meets maritime end-user accuracy specifications, and the model is transferable for integration into a cloud digital twin. Ongoing investigations aim to achieve comparable SoH prediction accuracy using only instantaneously measured variables, voltage, current, temperature, and features derived thereof eliminating the need for persistent storage of accumulated quantities in operational deployment.

Towards Differentiable, Machine-Learning-Accelerated Battery Simulations Across Scales

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Battery behavior emerges from tightly coupled phenomena spanning electronic, atomic, mesoscopic, and cell-level scales, yet these regimes are still largely modeled in isolation. In this talk, I will present a vision for machine-learning-accelerated simulation frameworks that not only speed up models across scales, but also render them differentiable and composable as a single end-to-end object for cross-scale optimization. I will discuss our progress in building surrogate and generative models for electronic-structure and atomistic simulations, as well as recent efforts to accelerate or replace phase-field models at the mesoscale and multiphysics cell-level models at the macroscale. Together, these developments point toward a new paradigm for batteries: differentiable multiscale simulation pipelines that enable rapid design, inverse modeling, and optimization across the full hierarchy of battery physics.

Electrolyte motion induced solid-phase lithium inhomogeneity in lithium-ion batteries

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Electrolyte motion induced salt inhomogeneity (EMSI) has been linked to capacity fade mechanisms such as lithium plating in lithium-ion cells, yet the liquid-phase salt gradients represent only the initial consequence of electrolyte motion. How EMSI ultimately translates into performance loss remains poorly understood. Here, we extend a previously developed modelling framework, incorporating electrolyte flow and electrode mechanics in an 18650 cylindrical cell, to decouple kinetic, transport and thermodynamic overpotential contributions, and trace the causal chain from salt redistribution to capacity fade. We show that EMSI-driven salt gradients propagate into persistent solid-phase lithium inhomogeneity in both positive and negative electrodes, causing uneven utilisation along the cell axis that manifests as apparent capacity fade, an effect further accentuated by the anode overhang near the electrode edge. By mapping the onset of lithium plating across a range of operating conditions, we demonstrate that plating susceptibility is governed by the interplay of liquid- and solid-phase concentrations and is significantly amplified by the mechanical constraints in the wound jelly roll. We reveal that the strong concentration dependence of electrolyte viscosity introduces an intrinsic asymmetry in salt redistribution: protocols with unequal charge and discharge rates produce a direction-dependent inhomogeneity that vanishes when viscosity is treated as a constant. These findings establish design guidelines for mitigating EMSI and underscore the necessity of accounting for electrolyte motion when optimising cell architecture and cycling protocols.

Modeling Ion Transport in Solid-State Electrolytes: From the Perspective of Potential Energy Surfaces

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Ion transport in solid-state electrolytes limits the performance of safe, high energy density solid state batteries. Improving these materials requires reliable predictions of ionic conductivity and mechanistic insight into how chemistry, structure, and disorder control ion diffusion, which in turn demands efficient modeling approaches that overcome the time and length scale limitations of molecular dynamics.

In this talk, I will present our work on cost efficient multiscale tools for modeling ion diffusion in solid state electrolytes. The approach applies topological and geometric analysis of the potential energy landscape to identify ion sites, diffusion pathways, and transport bottlenecks, and couples this with efficient statistical models to predict ionic diffusivities in electrolyte materials with ab initio molecular dynamics accuracy at a fraction of the computational cost. The framework also generates physically interpretable energy landscape descriptors – such as migration barrier distributions and network connectivity – that directly connect structure to ionic transport and performance, and enable physics based machine learning models for accelerated materials discovery.

I will further discuss insights from our calculations, including the effects of ion substitution and configurational entropy on the effective free energy landscape for lithium transport, and outline ongoing efforts to extend this methodology to non crystalline electrolytes e.g. polymer based systems and multiphase composites.

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Multi-scale degradation modelling of lithium-ion batteries.

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Empirical stress-factor models are widely used to estimate lithium-ion battery aging in mobility and stationary applications, expressing capacity fade as a function of temperature, state of charge, depth of discharge, mean state of charge, and charge/discharge currents. Such models are parametrized at the cell level and extrapolated to module and pack scales under the implicit assumption of uniform stress across all cells. This assumption neglects thermal gradients, cell-to-cell parameter dispersion, and current redistribution effects that emerge at module and pack scales. The accuracy of this extrapolation has not been systematically quantified for Nordic mobility duty cycles. This work compares three structurally different aging models for a large-format NMC pouch cell a physics-based pseudo-two-dimensional model with SEI growth, lithium plating, and loss-of-active-material submodels implemented in PyBaMM; an equivalent circuit model parametrized from impedance and pulse-current measurements; and a published empirical stress-factor model under identical operational profiles at cell, module, and pack scales. Module and pack simulations are conducted in LIIONPACK with realistic cell-to-cell parameter dispersion and lumped thermal coupling. The cross-model comparison quantifies the extrapolation error of cell-level empirical aging models when applied at pack scale and identifies operating regions where physics-based multi-scale modelling is required for reliable lifetime prediction.

Entropy Sinks the Convex Hull in Sodiated Black Phosphorus

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The development of Na-ion batteries (NIBs) is one route to practical, utility-scale energy storage with improved scalability and energy security, relative to Li-ion batteries (LIBs), especially within Europe and Canada. However, the intercalation-based graphite negative electrodes that provide LIBs such exceptional lifetime are fundamentally incompatible with NIBs, because Na intercalation in graphite is endergonic. Black phosphorus is structurally analogous to graphite, but does electrochemically intercalate Na, making it a potential alternative. Insertion electrodes (of which intercalation electrodes are a subset) are known to have a significant entropy contribution due to the large number of possible geometric configurations. The purpose of this work is to evaluate the significance of configurational entropy for DFT energy calculations of sodiated black phosphorus (NaxP) electrodes. For these calculations, B86bPBE-XDM(Z) is used to include accurate representation of the interactions between adjacent black phosphorus layers, as well as intercalated Na atoms. Experimental measurements, such as temperature-dependent electrode potentials and isothermal microcalorimetry, are used to measure the entropy during sodiation of NaxP, for $x \leq 0.5$. The results show that including configurational entropy decreases the energy of some stoichiometries below what is expected for the convex hull based on a single Na configuration. The implications of this work suggest new computational approaches are needed for properly determining the true convex hull of insertion and intercalation electrodes, which make up the vast majority of battery electrode materials.

In situ monitoring of Lithium-ion Battery Health Using Acoustic Emissions

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Lithium-ion batteries (LIBs) are essential for electric vehicles, consumer electronics, and large-scale energy storage systems. Reliable battery health monitoring is therefore critical for ensuring safe operation, optimizing performance, and supporting second-life applications. Conventional diagnostic methods, such as voltage and current profiling or electrochemical impedance spectroscopy, provide useful information but often require offline analysis, direct electrical connections, or controlled testing conditions, limiting their use for real-time monitoring.

Acoustic emission (AE) technology offers a promising non-destructive approach for in-situ detection of LIB degradation. By capturing mechanical waves generated during battery operation, AE can provide insight into internal structural changes, including electrode cracking, gas formation, and electrolyte leakage. In this study, AE was applied to investigate degradation mechanisms in graphite/Li and NMC/Li coin cells assembled with $LiPF_6$ in EC:DEC electrolyte. A differential wideband sensor was attached to the cell surface to record acoustic signals. Identical cells were aged under similar conditions for validation.

The results showed significant graphite exfoliation at the fully charged state, with AE amplitudes reaching approximately 65 dB. Incremental analysis indicated that the highest AE amplitude occurred near the phase transition point, suggesting a strong correlation between acoustic signals and electrode structural changes during cycling. Further experiments on commercial LIBs were performed using a specially designed foam enclosure to reduce background noise. Initial findings indicate that AE signals related to microcracking can serve as distinct markers of electrode degradation.

Overall, this study demonstrates the potential of AE as a real-time, non-invasive diagnostic tool for monitoring LIB health and aging mechanisms.

Novel quantification techniques for electrolyte motion induced salt inhomogeneity in aged battery electrodes

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Electrolyte motion induced salt inhomogeneity (EMSI) has recently emerged as an important degradation mechanism in commercial lithium-ion batteries under fast-charging conditions.[1] During cycling, electrolyte redistribution can create salt concentration gradients across the cell, leading to local variations in ionic conductivity, and degradation behavior. However, directly measuring these inhomogeneities remains challenging due to the limited spatial resolution and complexity of existing techniques.

In this work, two complementary methods are presented to investigate and quantify EMSI in commercial lithium-ion batteries. First, an in-house developed impedance-based technique was used to locally quantify electrolyte salt concentration in extracted electrodes using dilution of residual salt and a custom multi-wire impedance probe. Second, an ex-situ micro X-ray fluorescence (μ-XRF) method was developed to directly map salt distributions across full electrodes by using $LiAsF_6$ as a tracer salt and calibrating the arsenic signal to local salt concentration.
Both methods revealed pronounced centimeter-scale salt gradients and tab-correlated inhomogeneities during cycling, demonstrating that EMSI in large-format cells is significantly more spatially heterogeneous and more strongly coupled to local pressure inhomogeneities than previously recognized, with important implications for commercial cell design and fast-charging strategies.

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Harvesting chemical aging data from batteries with gas sensors

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In order to optimize the life cycle of a lithium-ion battery (LiB), the path-dependent aging mechanisms and state of health of the battery must be known and understood [1,2]. Novel chemical data, such as specific gas profiles from inside the battery during its operation, can be helpful for improving the battery analytics and modeling.

Aging of LiBs involves gas evolution reactions linked to the degradation of the battery materials. Interesting gases marking cell aging and degradation are e.g. carbon dioxide (CO2), carbon monoxide (CO), ethylene (C2H4) and hydrogen (H2) [3]. Use of chemical gas sensors to collect the chemical information from batteries is still in early stages mainly focusing on venting gases and pack safety [4].

In our current work, we are developing a set-up integrating gas sensors in contact with the internal environment of the battery to measure aging related gas evolution. The aim is to provide data for improved aging models and enhance the safety of batteries. The set-up will be applicable to various battery chemistries, thus promoting battery development, safety and 2nd life use.

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Isothermal microcalorimetry techniques for assessing battery degradation: Theory and application

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Isothermal microcalorimetry paired with electrochemical testing has been established as a powerful technique for gaining insights into degradation of battery cells. Thermal signals belonging to parasitic reactions that occur during battery operation provide key degradation parameters that cannot be determined from electrochemical cycling along. This talk will provide an introduction to the Battery Cycler Microcalorimeter Solution, and give an overview into the unique insights into battery degradation this technique provides.

$Li_3OCl|Li$ Interfaces for Solid-State Batteries: A Defect-Engineering Study

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The performance of solid-state lithium-metal batteries is critically influenced by the interface between the solid electrolyte and lithium metal. Li_3OCl antiperovskite electrolytes offer attractive ionic transport properties, yet their application is limited by interfacial instability and suboptimal lithium transport. In this study, we investigate the $Li_3OCl|Li$ interface using first-principles calculations, with a focus on defect engineering in the Li_3OCl solid electrolyte. Explicit atomistic interface models are constructed to examine interfacial structure, energetics, and charge redistribution. Intrinsic lithium defects are introduced to assess their impact on bulk and interfacial behavior. The results show that defect engineering can significantly improve lithium affinity and reduce interfacial energy while enhancing ion transport pathways and maintaining electronic insulation. These findings provide practical atomic-scale insights into stabilizing $Li_3OCl|Li$ interfaces and highlight defect engineering as an effective strategy for advancing solid-state lithium-metal battery technologies.

Nano-confinement engineered glassy MOF electrolytes for high-performance lithium metal batteries

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Composite-solid-state electrolytes (CSEs) hold significant promise for the practical application of lithium metal batteries (LMBs). However, insufficient interfacial coupling between polymer matrices and inorganic fillers results in heterogeneous ion-transport pathways, space-charge, and mechanical discontinuity, thereby limiting Li+ mobility and electrochemical stability. Herein, we report a nanoscale-confined polymer electrolyte constructed within a glassy metal-organic framework, establishing an isotropic, grain-boundary-free ion transport network with enhanced mechanical robustness and intrinsic nonflammability. The resulting electrolyte exhibits rapid Li+ transport, delivering a high ionic conductivity of 1.2 × 10−3 S cm−1, and an elevated lithium-ion transference number (tLi+) of 0.74, together with excellent tensile strength and elongation (1.2 MPa and 167%, respectively). Symmetric Li||Li cells demonstrate stable Li plating/stripping for up to 1600 h at 0.2 mA cm−2, while Li||LiFePO4 cells maintain long-term cycling stability over 900 cycles at room temperature. Benefiting from a wide electrochemical stability window of up to 5.1 V, Li||LiNi0.8Co0.1Mn0.1O2 cells deliver stable cycling over 240 cycles at 2 C under 4.2 V and maintain stable operation for 100 cycles at an elevated cut-off voltage of 4.4 V, highlighting the robustness of the electrolyte under high-voltage conditions.

Polymer-based electrolytes for solid-state batteries, addressing energy density, safety and sustainability

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Adoption of all-solid-state designs by polymer materials, ceramics, low-volatility additives, and hybrids thereof represent a promising solution towards next-gen, advanced alkali metal (Li, Na)-ion secondary batteries; in addition to safety advantages, these offer higher energy density and longer runtime than traditional Li-ion batteries. However, low ionic conductivity, low cation transport properties and issues in sustainable and scalable manufacturing processes must be overcome for market deployment.
Herein, recent advancements in polymer-based electrolytes with high ionic mobility, designed for safe and efficient solid-state batteries, are highlighted. Polymer matrices include poly(ethylene oxide), poly(carbonates), poly(vinylidene fluoride), and various blends thereof. Sustainable techniques, including solvent-free extrusion and UV-induced photo-polymerization, are used for solid electrolyte production. Incorporating room-temperature ionic liquids, low-volatility additives, and biosourced materials further improves electrochemical performance, achieving near-theoretical capacities at high C-rates with stable cycling at ambient conditions, also in combination with high-energy 4V class cathodes. Single-ion conducting polyelectrolytes are also particularly promising as they feature immobilized anions and free-to-move lithium counterions, resulting in a lithium transference number close to unity and resistance towards dendrite growth. Eventually, in terms of sustainable development, the aim is at exploring alternative recycling pathways for materials holding potential for a second life within the energy storage domain, particularly as components in advanced solid-state batteries.

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Synthesis of asymmetric sodium spiroborate monomers for single-ion sodium conducting polymer electrolytes

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Single-ion conducting polymer electrolytes (SICPEs) are promising new materials which can reduce dendrite formation and increase charging speeds in sodium ion batteries. In these polymer electrolytes, the anion is chemically bonded to the polymer matrix, leaving only the cation mobile. Like in most alkaline metal batteries, the most explored salts are highly fluorinated, complicating recovery and recycling of the materials due to safety and environmental hazards. Here, we aim to design fluorine-free spiroborate monomers which can then be polymerized into SICPEs for use in sodium batteries. This is accomplished by first synthesizing asymmetric anions. Various methods are explored to favor the formation of the asymmetric anion over the symmetric versions. The anions are then modified with methacrylate to render them polymerizable. The spiroborate monomers are copolymerized with polycaprolactone to form polymer electrolytes. Results will include the optimized synthesis and polymerization conditions of the monomers as well as their electrochemical properties and performance in SICPE solid state sodium batteries. The salts and monomers are characterized by nuclear magnetic resonance spectroscopy (NMR) and mass spectroscopy (MS). These findings can contribute to the development of new polymer electrolyte materials for safer and more sustainable sodium battery technologies.

Nanocellulose Fibril-Templated Preparation of Na1+xZr2SixP3-xO12 (NZSP) NASICON Electrolytes

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Solid-state electrolytes (SSEs) can address the issues of safety, longevity, and energy density limitations in batteries, but an up-scaling challenge remains from high-risk processing parring with good ionic conductivity and interfacial contact.

Meanwhile, NASICON-type SSEs for sodium-ion batteries have been investigated widely for achieving a decent balance of stability for performance. Their progress nonetheless is still hampered by non-uniform structural design and impurity apparitions which reduces the Na+ ion transport efficiency.

Our group introduces cellulose nanofibrils (CNFs) as a biotemplate [3] for the arrangement of $Na1+xZr_2SixP3-xO_{12}$ ($0 \leq x \leq 3$, NZSP) electrolytes. The CNF's 3D fibre network permits the passage of NZSP sol, creating a systematic alignment of the NASICON grains. Material characterisation reveals a solid solution ($x \sim 2.4$) consisting of monoclinic and rhombohedral NZSP crystals, with the CNF-templated NZSP favouring the latter. X-ray diffraction (XRD) and scanning electron microscopy (SEM) results reveal a reduction of impurities and more uniform NZSP grains from the CNF-NZSP.

Sintered CNF-NZSP pellets show higher ionic conductivities (~3×10^-4 S cm-1, 25ºC) compared to regular NZSP pellets, rendering them better candidates for NASICON-type SSEs. This work aims to determine the magnitude of ionic conductivity improvement and reduction of interfacial resistance with biotemplated NASICON SSEs. Alongside, this work has the potential to increase the valorisation of biomass components in energy storage application, speeding up the realisation of solid-state, sodium-ion batteries.

Insights into the electrochemical performance of hard carbon from wood in Na-ion battery negative electrodes

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Sodium-ion batteries (SIBs) are now being commercialized and are already beating lithium-ion batteries when it comes to safety, low-temperature performance, sustainability and cost. One of the most important advantages of SIBs is that they can be made from abundant raw materials in a low-energy process. The state-of-the-art negative electrode is the clearest example. Hard carbon can be made from any type of biomass and is synthesized at considerably lower temperatures and holding times than graphite.

Cellulose and lignin are the most abundant organic compounds on Earth, and in the Nordic countries there is more than enough wood to supply the world's need for batteries. Hard carbon from wood has shown great potential with high capacities and a very high initial coulombic efficiency, which is important in full cells. In this study, wood from different types of trees, as well as leaves, have been used as precursors. To understand the electrochemical properties of hard carbons from different types of wood precursors, electrodes have been made with hard carbons from various combinations of cellulose and different types of lignin. The hard carbons are characterized by XRD, nitrogen adsorption, particle size distribution and SEM. Electrodes made from these hard carbons have been subject to rate performance tests and continuous cycling over 500 cycles, and differences in the electrochemical cycling properties are correlated with the physical properties.

ALD Al2O3 artificial SEI for improved stability of porous silicon anodes

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Silicon (Si), as one of the most promising anode materials, has attracted significant interest for next-generation lithium-ion batteries (LIBs), owing to its extremely high theoretical capacity [1]. However, its practical application is hindered by severe volume expansion/contraction and unstable interfacial reactions during cycling. In this work, we focus on interfacial stabilization of mesoporous Si, in which the pore structure accommodates volume expansion through an artificial solid electrolyte interphase (SEI) formed via atomic layer deposition (ALD). Porous silicon powders were prepared by electrochemical etching of Si<100> wafers, followed by peeling, milling, and sieving to 10-25 µm. The powder surfaces were then modified by ALD to form conformal ultrathin Al2O3 coatings as artificial SEI layers, with varying numbers of ALD cycles (TMA+water regime) to tune the coating thickness. X-ray photoelectron spectroscopy confirmed the formation of Al2O3 on the surface of powders, evidenced by the characteristic Al-O signal in the O 1s spectrum. Electrochemical results show that ALD-coated samples exhibit improved initial columbic efficiency (ICE) compared to the uncoated sample, while rate performance shows a non-monotonic dependence on coating thickness. Notably, the sample with 5 ALD cycles (~0.5 nm thickness) delivers the best balance between higher ICE and improved capacity retention. Further work will focus on elucidating the underlying stabilization mechanisms.

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Entropy, Electrolytes and Electrodes

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It has become a trend in the battery field to talk about designed or engineered electrolytes and electrodes – and not seldom this is combined with the "buzzword" entropy. The very role of entropy is, however, far from often clear – or perhaps not even present in the materials.

We have now during the last 5-6 years, created and studied in details a wide range of both low, medium and high entropy electrolytes and electrodes for really try to outline/probe the possible role of entropy for observed properties – alongside impressive performance.

Basically, high-entropy alloys (HEAs) have their main feat in that they (ideally) are more mechanically stable, i.e. show improved cycling stability for the conversion-alloying reactions, than conventional battery alloy anode materials, while high entropy electrolytes, most significantly molten salt electrolytes (MSEs), which can be stepping-stones towards completely solvent-free and semi-solid room-temperature electrolytes, have uniquely modified local structure and dynamics. There is much to learn from these early proof-of-concept studies that hopefully also can be transferred to next generation battery chemistry and technology.

The "smörgåsbord" I provide will most hopefully induce some order in the entropy!

EFFECT OF CALCINATION ON FULL-CELL PERFORMANCE OF P2-NaxFe1/2Mn1/2O2 CATHODE

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The effects of calcination temperature, duration, atmosphere, and Fe0.5Mn0.5CO3 precursor1 particle size on the sodium-ion battery cathode P2-NaxFe1/2Mn1/2O2 were investigated in full cells paired with commercial hard carbon. The calcination reaction was studied using thermogravimetric analysis and high-temperature X-ray diffraction. The results indicate that the formation of layered P2 oxide proceeds through intermediate metal oxides formed from the carbonate precursors. Optimized long-term cycling performance was achieved without pre calcination by employing an oxygen atmosphere, a calcination temperature of 850 °C, and a calcination time between 0 and 6 h. Additionally, the influence of the negative to positive (N/P) capacity ratio on full cell performance was examined. N/P ratios close to 1.0 delivered higher initial capacities, while higher ratios up to 1.4 enhanced long term cycling stability. The effect of anode slurry compositions 80:10:10 and 96:00:04 was also evaluated. The results show that the 96:00:04 composition, which excludes conductive carbon, yields higher capacity. This improvement is attributed to the reduced surface area, resulting in lower sodium consumption for solid electrolyte interphase formation during the initial cycles.

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Layered Oxide Cathodes with Ambient Processing for Potassium-Ion Batteries

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Potassium-ion batteries are attracting increasing interest as sustainable alternatives to lithium-ion systems owing to the abundance of potassium, low material cost, high liquid-electrolyte ionic conductivity, and compatibility with graphite-based anodes. Layered manganese oxides are particularly promising group of cathode materials because they combine low-cost transition metals with high operating voltage and scalable synthesis. However, most reported K-layered oxide cathodes are processed under dry-room or glovebox conditions, limiting their practical manufacturability. Here, we investigate ambient-processed K0.5MnO2 cathodes for potassium-ion batteries and evaluate how air exposure, electrolyte formulation, and cell design affect their structural stability and electrochemical performance.

K0.5MnO2 was synthesized by a solid-state route and deliberately processed under ambient conditions. Structural and surface changes induced by air exposure were examined using X-ray diffraction, X-ray photoelectron spectroscopy, and Raman spectroscopy, revealing the sensitivity of the layered oxide framework and surface chemistry to moisture and atmospheric species. The electrochemical behavior was then studied in potassium half-cells using KTFSI-based electrolytes with different solvent systems, including TEGDME and EC/DEC, to identify electrolyte environments that improve reversibility and cycling stability. Rate capability, capacity retention, and long-term cycling were further assessed to determine strategies for increasing the reversible capacity of ambient-processed cathodes. Finally, the optimized cathode/electrolyte combination was evaluated in full-cell configurations to examine its practical relevance beyond half-cell testing.

Developing zwitterionic binder systems for water-processable lithium-ion battery cathodes with high voltage stability

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Most commercial lithium-ion batteries rely on polyvinyl difluoride (PVDF) binders despite increasing demands for sustainable manufacturing and improved safety. The environmental risks associated with polyfluoroalkyl substances (PFAS) and the need for toxic solvents to process fluorinated binders have motivated the search for alternative binding concepts with greener profiles.

This work investigates zwitterionic polymer binders as water-processable, fluorine-free alternatives to PVDF. The polymers incorporate both cationic and anionic functional groups, enabling aqueous electrode processing while promoting ionic coordination with lithium ions and strong adhesion to metal oxide particles and current collectors. These interactions are expected to enhance electrode integrity and reduce interfacial resistance. Zwitterionic polymers have previously demonstrated potential as solid electrolyte materials, raising the possibility of multifunctional binder–electrolyte systems for next-generation lithium-ion batteries.

The presentation outlines the journey in design and development of zwitterionic binder materials, including evaluation of solubility, mechanical properties, ionic transport, and electrochemical stability. The study establishes structure–property relationships governing binder performance and demonstrates how binder chemistry can improve the electrochemical battery performance as well as the environmental profile of lithium-ion batteries.

Improving the performance of solid boosters in flow batteries

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Aqueous flow batteries are promising approach for large-scale stationary energy storage, but storage capacity is limited by solubility of the redox active species. The capacity can be increased by incorporating solid redox active materials into the tanks as solid boosters. Now, the solids are charged or discharged in a chemical reaction with the flow battery electrolyte.

We have investigated ferri/ferrocyanide electrolyte coupled with Prussian Blue in different conditions in the lab scale. We will discuss how modifying the experimental conditions allows achieving >70% utilization of the solid capacity. However, the system performance was still limited by slow charging/discharging of the solid. To better understand the limiting processes, we have utilized finite element modelling considering both the flow battery cell and the tank filled with solids to evaluate how different parameters affect the system performance and how the solid materials should be selected and formulated to reach high capacity utilization also at high current densities. The model was first validated against experimental data. Better capacity utilization can be obtained with increasing residency time of the electrolyte and decreasing the size of the solid particles.

Design and Advanced Characterization of Aqueous Na- and Zn-Ion Battery Materials

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Aqueous insertion batteries offer a safe, sustainable, and low-cost alternative to conventional Li-ion systems for large-scale stationary energy storage. However, practical scale-up is hindered by narrow electrochemical stability windows and severe electrode degradation driven by the complex acid-base chemistry of aqueous mediums. To address these challenges, this work utilizes a comprehensive multi-technique synthesis and characterization approach to investigate framework-structured NASICON and Prussian Blue Analogue (PBA) materials. For the negative electrode, NASICON-type $NaTi_2(PO_4)_3$ (NTP) suffers from parasitic reactions causing self-discharge and degradation. Through operando local pH monitoring combined with solid-state NMR, XRD, and EDX, we demonstrated that both hydrogen evolution (HER) and oxygen reduction (ORR) drive a pH increase during cycling. While HER is negligible under mildly alkaline conditions, chemical ORR, driven by O_2 reacting with Ti(III), dominates. Crucially, capacity fade stems primarily from electronic contact failure caused by the growth of amorphous $TiO(OH)(H_2PO_4)\cdot nH_2O$ interphase layers, rather than bulk NTP decomposition. Managing local oxygen concentration and pH enables highly stable NTP operation in low-concentration aqueous electrolytes. For the positive electrode, Zn-rich PBAs like $Zn_2[Fe(CN)_6]$ were studied for zero-excess-metal-free (anode-free) aqueous Zn-ion batteries. We elucidated synthesis–structure–property relationships by focusing on phase formation, Fe(II/III) oxidation states, and structural hydration, with operando XRD revealing previously unreported phase evolution during synthesis and cycling. Together, these findings provide critical insights into degradation mechanisms and mitigation strategies, unlocking the potential of stable, high-efficiency aqueous battery systems.

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Automated development of PFAS-free aqueous electrolytes for Na-ion batteries

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Developing safe and sustainable electrolytes is a critical hurdle for next-generation batteries. Commercial systems rely on flammable organic solvents and fluorinated salts (e.g., LiPF6), which, while forming stable interphases, pose significant fire risks and release toxic hydrofluoric acid (HF). Furthermore, tightening PFAS regulations and high dry-room manufacturing costs necessitate moisture-tolerant, PFAS-free alternatives.

This work addresses these challenges by exploring High-Entropy Electrolytes (HEEs) within aqueous systems. While water-based electrolytes are intrinsically safe and cost-effective, they typically suffer from a narrow Electrochemical Stability Window (ESW). By leveraging the complex solvation structures of multiple salts, HEEs can widen the ESW while maintaining high ionic conductivity.

To navigate the vast, high-dimensional design space of HEEs, we developed an automated electrolyte development platform integrating high-fidelity characterization with Bayesian Optimization (BO). This system enables the autonomous profiling of 24 electrolytes per day across a 0–40°C range. Utilizing a three-electrode cell (Pt electrodes and Ag/AgCl reference), the platform performs Electrochemical Impedance Spectroscopy (EIS) and Linear Sweep Voltammetry (LSV) to measure ionic conductivity (mS cm^{-1}) and ESW (V).

Through high-throughput screening, we identified optimized combinations of NaAc, NaNO3, and Na2SO4 that achieve the stability required for practical galvanostatic cycling. This automated approach accelerates the discovery of PFAS-free formulations, bridging the gap between environmental sustainability and the rigorous performance demands of next-generation energy storage.

Revisiting spiroborate salts beyond bis(oxalate) borate as fluorine free electrolytes for sodium ion batteries.

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Design to recycle is a demanding requirement for next generation secondary alkaline-ion batteries. Fluorine containing compounds in both electrodes and electrolyte complicate recycling and increase environmental risks due to the possible formation of hazardous substances such as HF and PFAs. Younesi and co-workers introduced bis(oxalate)borate electrolytes for sodium ion batteries (SIB) as a promising route toward fluorine free high performance electrolytes[1]. However, this suffers from limited solubility in most solvents and a tendency to form a resistive solid electrolyte interphase (SEI).

Nevertheless, it opens for the possibility to explore a wide range of related compounds by modifying the ligands at the boron centre in order to tailor electrolyte properties. While many spiroborate compounds have previously been investigated for Li ion batteries, they were primarily considered as film forming additives rather than as electrolyte salts. In this study, we analyse several fluorine free spiroborate electrolytes based on diol or hydroxy acid ligands and analyse their physicochemical and electrochemical properties as well as their electrochemical performance in sodium-ion full cells. The salts were synthesized using an adapted, simple azeotropic distillation approach. Using bis(salicylato)borate as a case study, we demonstrate that substitution on the aromatic ring not only shifts the electrochemical stability window but also dramatically improves salt solubility.

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The role of electrified hydrometallurgical unit processes in Li-battery recycling

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Li-battery recycling can be conducted either by pyro-hydrometallurgical or solely hydrometallurgical refining routes. Hydrometallurgical processing includes extraction and purification in aqueous media, with a typical flowsheet consisting of leaching, neutralization, separation, solution purification, and metal recovery unit processes, as well as lixiviant recirculation. Most of the unit processes have traditionally been chemically driven, including the use of acids (leaching), alkaline chemicals (neutralization), organic chemicals (extractants, diluents, modifiers in solvent extraction), precipitation agents (impurity removal, metal recovery, wastewater purification) as well as ion exchange resins when applicable. However, electrified unit processes have been stated as one of the twelve principles of circular hydrometallurgy, as they may provide competitivity in several aspects of sustainability, when coupled with use of low-carbon electricity.

In battery recycling, the most typically suggested electrometallurgical process is electrowinning i.e. recovery of solid metal on cathode from highly purified solutions (after solvent extraction), while generating oxygen at the anode. However, interest in alternative electrified operations has recently grown, and several novel technologies as well as process flowsheets are emerging. Examples include direct electrowinning, anodic methods, synergistic cathodic–anodic recovery routes, pulsed methods as well as electrically driven lixiviant circulation. In electrified processes, chemical consumption decreases as a trade-off for electricity. Potentially, also waste generation may be decreased when e.g. Na_2SO_4 generation is avoided. Consequently, electrification—together with both incremental and disruptive process innovations, as well as digitalization—has potential to accelerate the decarbonization of battery industry.

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An investigation on the pyrolysis, flotation and leaching for the recycling of spent lithium-ion batteries

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The recycling of lithium-ion batteries (LIBs) has become one of the main research areas in battery value chain to meet the increasing need for their raw materials. Pyrolysis and flotation are alternative pre-treatment processes to be used prior hydrometallurgical leaching and the consequent battery materials recovery. Nevertheless, the advantages and barriers of integrated utilization of pyrolysis and/or flotation have not been systematically investigated. In this experimental study, various scenarios of pyrolysis, flotation and leaching were combined for the treatment of industrially produced black mass retrieved from spent batteries. The results showed that pyrolysis improved the separation efficiency of graphite from lithium metal oxides by aiding the liberation of particles from the binder. The graphite purity in flotation concentrate increased from nearly 60% to 80% despite the negative impact in the recovery from 60 % to 50%. Moreover, pyrolysis also increased the leaching yields of the metals from 40% to more than 80%. In addition, application of flotation prior to leaching increased the leaching yields of Ni and Co approximately 5%. It was found that higher dissolution yields of metals from the black mass can be achieved with the combination of pyrolysis and flotation before leaching. This trend was not observed for Li, possibly due to its partial dissolution in process water during flotation. The current study shows that optimization and integration of new alternative pre-treatment processes may improve process efficiency and help to build the most efficient pre-treatment strategies for LIB recycling.

Insights into the pre-treatment of spent LFP (LiFePO4) EV batteries for direct recycling purposes

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Recycling of Li-ion batteries (LIBs) is a hot research topic among academic and industrial researchers. Especially for low-cost LIB chemistries, such LFP (LiFePO4), direct recycling has become a popular strategy due to its potential to recover active materials in their intact form, as compared to the more conventional recycling routes. There is already a vast number of publications reporting novel methods of relithiation of spent LFP cathode active material (CAM). However, there is much less focus on the pre-treatment steps that must be taken before obtaining the CAM in a form suitable for regeneration. At the same time, the pre-treatment process influences the purity and chemical/mechanical integrity of the recovered CAM, which can largely affect the electrochemical performance of the regenerated material.

In this work, we present our latest findings on 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, shedding new light on the choice of discharging method depending on the subsequent treatment strategy of the spent CAM. Further, we explore methods of delamination of the CAM from the aluminum current collector and 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.

Enabling Industrial-Scale Battery Recycling: Insights from an Innovation Fund Project

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This presentation explores how battery recycling technologies can be scaled from demonstration to industrial deployment, using Fortum's NEXT HYDROMET project as a case example.

The project, supported by the EU Innovation Fund and national funding, demonstrates how advanced recycling solutions can be brought to industrial scale and integrated into the European battery value chain.

The presentation focuses on practical lessons from the project, including the role of public funding, technology maturity requirements (TRL), and key considerations in scaling new solutions. It also reflects on the importance of recycling in securing the availability of critical raw materials in Europe.

Transport Numbers of Ion-Exchange Membranes in Divalent Sulfate Electrolyte Solutions for Lithium- Ion Battery Recycling Applications

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Recycling spent lithium -ion batteries (LIBs) is essential for addressing environmental and resource challenges through the recovery of valuable materials. Electrodialysis has emerged as a promising electro-membrane strategy for the selective recovery of resources from spent LIBs. In particular, the separation of metals from leaching solutions of spent LIBs using electrodialysis with ion-exchange membranes (IEMs) has been proposed as a route for LIB recycling. Ion transport in IEMs plays a critical role in determining the efficiency and selectivity of ions in electro-membrane processes. This study presents the first investigation of transport properties, including ionic transport numbers and water transference coefficients, of Ni (II) and Co (II) ions across commercial IEMs using NiSO4 and CoSO4 electrolyte solutions, relevant to electrodialysis applications and recycling of LIBs. The permselectivity analysis was employed for the analysis of new electric potential measurements across Selemion IEMs in contact with aqueous NiSO4 and CoSO4 solutions within the framework of non-equilibrium thermodynamics. The transport numbers obtained for Ni (II) and Co (II) ions in sulfate salt solutions were 1.000 ± 0.006 and 1.003 ± 0.008, respectively, indicating high membrane selectivity and near-ideal transport behavior for these divalent sulfates. The corresponding water transference coefficients were found to be 16 ± 2 and 15 ± 3. These findings highlight the importance of accounting for water transport in the design of electrodialysis for antisolvent recovery in hydrometallurgical recycling of LIBs. The presented method can further support the development of efficient membranes for specific electro-membrane processes.

The secret life of e-scooter batteries

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Shared mobility has recently become a B€ industry with ~260 million e-scooter rides taken in Europe 2024 alone. Actors such as Lime, Dott, and Voi have operated shared e-scooter (SES) & e-bike fleets for >7 years, and with these businesses becoming profitable, use is likely to further expand. Given this, it is relevant to consider ways of benchmarking SES battery performance, just as for any other electric vehicles. The automotive industry and customers benefit from standardised usage profiles, such as the Worldwide Harmonized Light-Duty Vehicles Test Procedure (WLTP), but at present no such profiles exist for SES. Furthermore, little is known about SES-specific battery ageing, partly due to lack of understanding of operating conditions, including representative load profiles, arguably having a significant impact on lifetime [1].

Here we approach the challenge of identifying SES battery usage and load cycle, relevant for both lifetime testing and performance benchmarking, by using high frequency voltage, current, and temperature data collected from 10 thousand commercial SES both during rides (> 15 million) and standby (>3 months accumulated operation). This way we can identify fleetwide distributions in C-rates, temperatures, rest times, and state-of-charge windows traversed, using the battery information format (BIF) [2]. Combining all above, we can tentatively give recommendations for representative test conditions and power profiles, similar to WLTP etc., enabling accurate lab-testing of ETW batteries and future vehicle improvements.

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Analysis of optimization strategies for utilization of second life BESS to achieve maximum savings

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Background
With the exponential growth in the stationary energy storage market for Li-ion batteries, there is a great potential for utilization of used EV batteries in stationary solutions. This will extend the lifetime of batteries, accompanied by a lower total carbon footprint over the lifetime. There are, however, a great deal of challenges with implementation of used EV batteries in stationary solutions, including state of health diagnostics and integration and control of the EV batteries, where functionality varies across EV battery types.

Results
In this project, second life EV batteries were repurposed, to investigate the potential for reuse as energy storage on three pilot sites, Lempäälä-talo, Trosvik school and Rudskogen Motor Centre. Two different EV batteries were utilized. In addition, the theoretical potential for savings on these pilot sites were studied. The three sites encountered different challenges, had a different set of boundary conditions and great variations in electricity production and consumption profiles.

Conclusions
For the two different EV battery types, it was possible to make an overall similar battery rack, where most of the design remains constant, and mainly software was adjusted to match differences between the EV battery types. Still, it was challenging to optimize and adjust to local conditions. The pilots highlighted that economic and operational performance strongly depends on local conditions such as electricity demand patterns, billing systems and regulatory frameworks, underlining the importance of context-specific implementation.

Electrolyte-dependent behaviour of cellulose nanofibril separators in zinc metal batteries

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The limited electrochemical stability window of aqueous based electrolytes for zinc metal batteries has motivated the exploration of nonaqueous systems based on organic solvents. In such system, zinc triflate ($Zn(OTf)_2$) is commonly employed as a salt together with organic solvents (e.g. $Zn(OTf)_2$ in dimethyl sulfoxide or acetonitrile solvents). However, the role of the separator is often overlooked, with glass fiber or polyethylene separators used by default. However, other separator materials can bring further functionality and also add sustainability aspects.

In this work, we report on cellulose nanofibril (CNF) films as separators for nonaqueous zinc metal batteries. While CNF-based separators have shown promising performance in aqueous systems, its compatibility with nonaqueous electrolytes remains largely unexplored. Here we explore the functionality of CNF-based separators with $Zn(OTf)_2$ in dimethyl sulfoxide electrolyte and aqueous $Zn(OTf)_2$ as comparison. The electrochemical performance is evaluated in comparison to commercial separators in both symmetric Zn/Zn and asymmetric Zn/Cu cells. The results reveal an electrolyte-dependent behaviour, where CNF separators exhibit different stability and transport characteristics depending on the solvent used. These findings indicate that separator-electrolyte compatibility plays a critical role in determining electrochemical performance. Overall, this work highlights the importance of considering separator materials beyond conventional choices and emphasizes electrolyte-separator interactions in the design of nonaqueous zinc metal battery systems.

Comparative Degradation Analysis of Lithium-Ion and Sodium-Ion Batteries with Graphite, Silicon–Graphite, and Hard Carbon Anodes

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The transition toward low-carbon energy systems and electric mobility has increased the need for efficient, durable, and reliable battery technologies. Lithium-ion batteries (LIBs) and sodium-ion batteries (SIBs) are among the most promising rechargeable systems for these applications; however, their long-term performance strongly depends on cell chemistry, electrode design, and operating conditions.

This study compares the degradation behavior of three battery chemistries: silicon–graphite/NMC811, graphite/NMC811, and hard carbon/$Na_2NiFeMnO_4$. The cells are aged under systematically varied operating conditions, including temperature, state-of-charge (SOC) window, and C-rate, to investigate the effects of these parameters on degradation pathways. Periodic electrochemical characterization is performed using incremental capacity analysis (ICA, dQ/dV) and hybrid pulse power characterization (HPPC).

The results are expected to support improved cell chemistry selection, lifetime prediction, and operating strategy development for next-generation battery applications.

UV-Crosslinked PEO–PEC polymer electrolytes with cyclic carbonate additives for room-temperature alkali metal batteries

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The realization of safe and high-performance metal batteries operating at room temperature requires electrolyte systems that overcome the intrinsic limitations of conventional poly(ethylene oxide) (PEO)-based solid polymer electrolytes, particularly their crystallinity-driven low ionic conductivity. Herein, we performed a solvent-free approach to fabricate a UV-crosslinked poly(ethylene oxide)-poly(ethylene carbonate) (PEO–PEC) salt-in-polymer electrolyte via melt compounding, hot pressing, and in situ photopolymerization, yielding a mechanically robust and structurally stabilized matrix [1-3]. To enhance ion transport and interfacial behavior, cyclic carbonate additives are incorporated as functional plasticizers within the crosslinked network, enabling modulation of polymer dynamics and ion coordination. Among these, 1,2-butylene carbonate demonstrates the most favorable performance, reducing the glass transition temperature and enabling stable lithium plating/stripping over extended cycling (>2300 h), while delivering near-theoretical capacity in LFP-based solid-state cells at room temperature [4]. In parallel, the versatility of the PEO–PEC backbone is being explored for sodium metal systems through tailored salt-additive combinations, revealing comparable trends in transport and interfacial stabilization [5]. These findings highlight a generalizable strategy for designing crosslinked polymer electrolytes with immobilized plasticizers, offering a scalable pathway toward safe and efficient alkali metal batteries.

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Kraft Lignin Fractionation Enables Structure–Property Control in Hard Carbon Anodes for Sodium-Ion Batteries

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Kraft lignin (KL) is an abundant yet underutilized bio-aromatic resource with strong potential as a precursor for hard carbon (HC) anodes in sodium-ion batteries (SIBs). However, its complex structure often limits control over the properties of the resulting carbons. The inherent heterogeneity of lignin leads to inconsistent material properties, reducing process control and hindering efficient lignin valorization. Refining lignin into more homogeneous fractions therefore offers a viable strategy to reduce this heterogeneity and enable improved modification of lignin characteristics for downstream applications.

In this work, KL was fractionated using aqueous ethanol to produce precursors with distinct molecular differences, providing a controlled method for generating HCs with tailored physicochemical properties. These precursor-level modifications enable systematic investigation of how lignin structural features govern HC structure and electrochemical performance. The results show that precursor-level lignin modification enables direct control over HC properties, allowing electrochemical performance to be linked to lignin structure and chemistry, rather than carbonization conditions alone. Specifically, variations in lignin molecular weight and compositional features were directly correlated with the structure and properties of the resulting HCs, with these parameters showing strong correlations with HC microstructure. By linking these lignin features to subsequent electrochemical behavior, the results establish targeted modification of KL as a rational pathway for controlling HC properties and optimizing performance in sodium-ion batteries.

High-Voltage Stability of Single-Crystal NCM811 Cathodes Enabled by Aqueous Binder

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While high-nickel layered oxides are vital for high-energy lithium-ion batteries, their application is often hindered by structural degradation and interfacial instability at elevated potentials. This study investigates how the electrochemical stability of single-crystal LiNi0.8Co0.1Mn0.1O2 (SC-NCM811) cathodes is fundamentally dictated by the binder-network architecture established during aqueous processing of a carboxymethyl cellulose (CMC) crosslinked with citric acid (CA). We demonstrate that the electrode drying temperature is a governing parameter that controls the dehydration-induced crosslinking density and the resulting electrode porosity. Optimizing this process is critical; electrodes dried at 70℃ exhibit superior structural integrity compared to those processed at elevated temperatures. SEM analysis pronounced particle cracking is observed after 100 cycles in the electrode dried at elevated temperature, while the electrode dried at lower temperature largely preserves its structural integrity, indicating temperature-driven degradation. Furthermore, XPS analysis indicates that drying temperatures drive significant surface reconstruction and interphase evolution. Specifically, elevated drying temperatures promote the formation of the inactive rock-salt NiO phase in fresh electrodes. In contrast, cycled electrodes processed at optimized temperatures exhibit a more stable cathode-electrolyte interphase (CEI), highlighting the critical role of processing conditions in governing the cathode degradation pathway. The optimized CMC-CA system achieves a remarkable capacity retention of 92.2% after 100 cycles at 4.5 V, significantly outperforming conventional PVDF-based electrodes (retention of ~80%), which suffer from severe capacity fade and electrolyte decomposition under identical conditions. This work highlights the potential of optimized aqueous binder processing as a practical route toward more sustainable manufacturing of high-energy Ni-rich cathodes.

Unraveling morphological and phase evolution in barley husk-derived silica during magnesiothermic reduction

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Silicon is a promising lithium-ion batteries (LIBs) anode material due to its high theoretical capacity (3579 mAh g-1), enabling high-energy batteries when its large volume change is managed [1]. Porous Si (PSi) derived from biogenic silica offers a sustainable route to mitigate this challenge by providing structural buffering and enhanced ion transport [2]. In this work, mesoporous silica derived from barley husk is used as a precursor for PSi production via magnesiothermic reduction (MgTR). The morphological and phase evolution during each processing step is systematically investigated. Cross-sectional characterization is performed using SEM, TEM, and EDS, supported by argon milling and ultramicrotomy for sample preparation. Phase-distribution analysis (Figure 1) reveals a progressive transformation of the porous structure during MgTR and subsequent post-treatment steps. After H2O-washing, the reduction mix exhibits distinct Mg-rich and Si-rich regions, indicating residual Mg-based reaction products and deep diffusion of Mg into the mesoporous silica framework. Subsequent HCl washing effectively removed Mg-rich phases, exposing Si-rich and O-rich domains, while simultaneously generating big pores. Final HF washing further eliminates residual oxides, resulting in a highly interconnected meso and macro silicon structure. This hierarchical porosity improves lithium-ion diffusivity and accommodates volume changes, enabling high-performance LIB anodes.
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Automated Screening of Redox-Active Metal Complexes for Flow Batteries Using Pipetting Robot and battery testing.

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The transition from fossil-fuel-based energy systems to renewable energy sources has intensified the demand for scalable and sustainable energy storage technologies capable of addressing the intermittency of renewable power generation. Among the available technologies, redox flow batteries (RFBs) have emerged as promising candidates due to their scalability, safety, and cost-effectiveness. However, the development of stable and efficient electrolytes remains a major challenge, largely because the discovery of suitable redox-active materials is time-consuming and labor-intensive. This work presents an automated high-throughput approach for accelerating the identification and screening of redox-active materials for aqueous flow battery systems using the Opentrons OT-2 pipetting robot. The robotic platform enables rapid and reproducible synthesis of up to 96 samples in a single run, significantly reducing the experimental time and chemical consumption compared with conventional laboratory approaches, which typically require larger quantities of raw chemicals and several weeks to produce equivalent datasets. Water-soluble metal complexes of various metals like Fe, Mn, Cu, Cr, Ni, etc with organic ligands such as EDTA, PDTA, DTPA, Goods ligand, etc have been synthesized due to the advantages of safety, cost-effectiveness, and eco-friendliness of aqueous-based electrolytes. The synthesized complexes were characterized electrochemically using a semi-autonomous miniature three-electrode cyclic voltammetry setup to identify promising redox-active candidates. Potent compounds exhibiting favorable electrochemical behavior were subsequently reproduced through conventional synthesis routes and evaluated in flow battery cells to assess their cycling stability. The results demonstrate that laboratory automation can substantially accelerate the discovery and optimization of electrolyte materials for next-generation aqueous redox flow batteries.

ZnO coating nano-hematite surfaces effect on kraft lignin-derived graphite structure for LIB's

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Background.

Kraft lignin is a promising biomass precursor for graphite production in Europe due to its high availability (≈100 million tons per year) and carbon content (50–60%), but it has low graphitization capacity. Iron oxide-based catalysts are typically used to enhance graphitization, but sulfur impurities in lignin significantly deactivate them. The incorporation of zinc oxide as a protective component into iron-based catalytic systems offers an effective strategy for suppressing sulfur poisoning and increasing the efficiency of catalytic graphitization.

Results.

Nano hematite was synthesized by hydrothermal method from $FeCl_3$ and urea. ZnO coated Fe_2O_3 from $Zn(NO_3)_2*6H_2O$ solutions of varying concentrations. The effect of increasing the ZnO/Fe_2O_3 ratio in the coating at a constant lignin/Fe_2O_3 ratio (experiments 1R–7), as well as increasing the total catalyst content in the mixture at a fixed ZnO/Fe_2O_3 ratio (experiments 4, 9, 10), on graphite morphology, structural parameters, and electrochemical performance was studied compared to commercial graphite (Fig. 1). Lignin mixtures were subjected to pyrolysis at 700°C followed by induction graphitization at 2500°C.

Conclusion.

At a constant lignin/Fe_2O_3 ratio, increasing the ZnO content in the coating improves the ordering of the graphite layers but simultaneously increases the proportion of graphene-like carbon, reducing the overall quality of the graphite as an anode precursor. In contrast, a higher catalyst content at the optimal surface zinc concentration (experiment 10) resulted in the formation of more ordered graphite structures and demonstrated high initial coulombic efficiency and specific capacity. Raman spectroscopy and XRD results are consistent with electrochemical characteristics.

Battery drying conditions and rate capacity retention

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This work aims to bridge the knowledge gap between electrode drying and battery performance by illustrating which drying parameters have the largest influence on the electrochemical performance of the battery. Reducing energy consumption during electrode drying is essential for improving the cost and sustainability of lithium-ion battery (LIB) manufacturing. Electrode drying and solvent recovery account for a significant proportion of total manufacturing energy demand, typically between 30–50% depending on the drying method and battery chemistry. Understanding the relationship between electrode drying conditions and rate capacity retention is important to evaluate electrochemical limitations of the battery at high C-rates. Rate capacity retention is a phenomenon where battery performance degrades at high cycling rates. Conventional industrial drying methods using heated compressed air were investigated using a custom-built drying rig that allows scaling results from lab scale research to industrial conditions. The main parameters investigated are drying temperature, air velocity, and electrode thickness.

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Fluorine-Free Sulfonate Ionic Liquids and Battery Electrolytes

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Abstract
We have developed a series of fluorine-free sulfonate-anion-based ionic liquids (ILs) and their corresponding electrolytes for battery applications. The ILs are synthesized via alkylation approach, using methane sulfonic and ethane sulfonic acids as anionic counterparts, combined with various heterocyclic cations, including alkyl pyrrolidinium, piperidinium, imidazolinium, morpholinium, and alkoxy pyrrolidinium (Figure 1). Also, Li+-conducting electrolytes were prepared by doping 20 mol% and 40 mol% of lithium salts of respective anions with neat alkyl pyrrolidinium-based ILs. Comprehensive physico-chemical, thermal and electrochemical characterization of the ILs and the electrolytes were performed to evaluate their suitability as electrolyte components. The thermal decomposition temperatures are 300-360 °C and the ionic conductivities 0.04-8.5 mS cm-1 at 25 °C. Furthermore, we gain a mechanistic understanding of ion transport and interactions through FTIR and NMR spectroscopy, highlighting the influence of the alkyl chain length of cations and the sulfonate functionality of anions. The alkyl pyrrolidinium-based ILs demonstrated wide electrochemical stability windows, high ionic diffusivities, and superior ionic conductivities, while the imidazolinium-based ILs exhibited the best thermal stability. Overall, these sulfonate-based electrolytes exhibit favorable chemical, thermal, and electrochemical stabilities, suggesting these materials hold a strong potential as alternative electrolyte components for next generation batteries.

Keywords: Fluorine-free electrolytes, ionic liquids, ion diffusivity, next generation electrolytes

Fluorine-free binders for NMC811 cathodes: isolating intrinsic stability from aqueous processing effects

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The transition toward sustainable lithium-ion battery manufacturing has increased interest in PFAS-free, water-processable electrode components. Replacing fluorinated binders like polyvinylidene fluoride (PVDF) in high-voltage cathodes such as $LiNi_{0.8}Mn_{0.1}Co_{0.1}O_2$ (NMC811) remains challenging, as fluorine-free aqueous binders lack sufficient stability. Aqueous processing further complicates this due to reactions between NMC811 and water, creating alkaline slurries that can corrode aluminium current collectors and degrade binders. Because fluorine-free materials and aqueous processing are often studied together, it remains unclear whether performance limitations arise from intrinsic binder instability or the processing conditions.

This work investigates the processability and electrochemical stability of fluorine-free, water-soluble cathode binders, with emphasis on isolating intrinsic binder behaviour and structure-property relationships from NMC811-induced effects and aqueous processes. These results are then compared to results from the more conventional PVDF binder which is processed using the toxic organic solvent N-methyl-2-pyrrolidone. Slurry acidification and the use of acidic binders are explored to control pH and enable efficient aqueous electrode fabrication. To further isolate binder properties, model electrodes free from NMC811 and instead based on glassy carbon are employed. The binder behaviour and stability are evaluated using different characterization and analysis techniques, such as electrochemical testing, ICP-OES and SEM.

This approach establishes a framework for systematic binder evaluation and supports the development of environmentally benign binders and processing strategies for high-voltage NMC811 cathodes.

Improving initial coulombic efficiency of biomass-derived hard carbon via structure and electrolyte engineering

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Biomass-derived hard carbon is a promising anode material for sodium-ion batteries, but its practical application is hindered by low initial coulombic efficiency (ICE) caused by irreversible sodium loss during the first cycle. In this work, hard carbons derived from wood-waste and peat were engineered through catalyst-assisted pyrolysis and evaluated in both carbonate and ionic liquid electrolytes to understand and mitigate first-cycle inefficiencies. Catalytic treatment increased local structural ordering and modified pore architecture by reducing microporosity and enhancing mesoporosity. As a result, ICE improved from 26% in untreated wood-waste carbon to approximately 41–42% after catalytic processing. Peat-derived carbons with optimized structure delivered capacities up to 192 mAh g^{-1} with an ICE of 67% in $NaPF_6$-based carbonate electrolyte. The electrochemical performance strongly depended on electrolyte chemistry: carbonate systems favored higher ICE, whereas ionic liquid electrolytes enabled higher reversible capacities (up to ~195 mAh g^{-1}), improved rate capability, and lower charge-transfer resistance. In addition, direct-contact pre-sodiation significantly increased ICE to 75% under optimized conditions. Electrochemical analyses indicate improved interfacial kinetics and predominantly surface-controlled sodium storage behavior in the engineered carbons. These results demonstrate that synergistic control of structure and electrolyte is an effective strategy to enhance ICE and overall performance of biomass-derived hard carbon, providing practical pathways for advancing sustainable sodium-ion battery anodes.

In situ ethanol-mediated growth of lithium indium chloride on lithium cobalt oxide cathodes

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All-solid-state lithium batteries require solid electrolytes with high ionic conductivity and seamless interfacial contact with the cathode. Halide electrolytes, such as lithium indium chloride (LIC), are promising candidates due to their high oxidative stability and intrinsic compatibility with 4V-class oxide cathodes like $LiCoO_2$ (LCO). However, achieving intimate solid-solid contact using traditional mechanical mixing remains challenging and limits cell performance. This study investigates ethanol-mediated liquid-phase synthesis for the in-situ growth of LIC directly on an LCO cathode using a spin-coating method to build continuous 3D lithium-ion conduction pathways and minimize interfacial resistance. Precursor solutions comprising LiCl and $InCl_3$ mixed in ethanol were spin-coated onto the LCO cathode and subsequently heat-treated at 200 °C for 12 h under argon to induce crystallization. X-ray diffraction (XRD) analysis was utilized to evaluate the phase evolution and purity of the coated layers. The XRD pattern for the spin-coated sample confirmed the successful formation of the desired LIC phase. Alongside the LIC peaks, the diffraction data also revealed the presence of unreacted LiCl and intermediate solvate peaks corresponding to $C_{15}H_{21}InO_6$.[1] The ethanol-mediated spin-coating approach demonstrates feasibility for depositing LIC onto LCO cathodes, facilitating in situ crystal growth. While the primary superionic halide phase successfully nucleates, the presence of residual LiCl and $C_{15}H_{21}InO_6$ solvates indicates further optimization of the post-treatment conditions, such as adjusting the 12 h heating duration or transitioning from argon to vacuum heating. Ultimately, this scalable wet-chemistry strategy holds significant promise for engineering superior cathode-electrolyte interfaces.

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Doped TiO2 flame spray produced nanoparticles for enhancing porous carbon cathode of lithium–sulfur battery

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Considered among the most promising next-generation energy storage technologies, lithium–sulfur batteries offer theoretical specific capacity of 1675 mAh/g and nearly double the energy densities compared to the lithium-ion battery. Still, the commercial application is limited by issues such as the polysulfide shuttle effect. Affordable metal oxides, such as TiO_2, could be used to bind the polar polysulfides, improving cell longevity by preventing the loss of active materials. However, this approach can suffer from the inherent poor conductivity of the metal oxides limiting cell performance. Based on computational studies, the electrical conductivity of TiO_2 could be greatly increased by doping with additional elements.[1]

In this work, doped TiO_2 nanoparticles synthesized by flame spray pyrolysis were used with porous carbon to improve the electrochemical performance of lithium sulfur battery cathode. Polar TiO_2 can serve as a host that chemically adsorbs lithium polysulfides, suppressing diffusion, and catalyzing redox reactions enhancing performance of Li–S cells.[2],[3] To investigate the effect of doping on the properties of the material, TiO_2 nanoparticles with antimony, zirconium and niobium doping were prepared. Properties of the prepared nanoparticles and composites were extensively characterized, and the electrochemical behavior was tested in coin cells.

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Prelithiation as a strategy to stabilize high entropy alloy anodes

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High entropy alloy (HEA) anodes have attracted attention as lithium-ion battery anodes, much due to their high specific capacities: 500-1300 mAh/g.[1,2] HEA anodes, however, in general suffer from poor coulombic efficiency and meaningful volume changes during cycling due to alloying/dealloying reactions, limiting their long-term stability.[2–4] The low coulombic efficiency is ascribed to both SEI formation and irreversible alloying reactions, which may be further exacerbated by the fact that HEAs are typically synthesized in un-lithiated state. To remedy this, we have synthesized HEAs in a pre-lithiated state using an existing one-step mechanochemical synthesis method.[1] We hypothesize that we thereby create a reservoir of Li useful for SEI formation.

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Sodium-ion battery Na-site doping: effects of metal ordering and defect engineering

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Sodium-ion batteries (SIB) offer an alternative to lithium-ion batteries (LIB). However, SIBs suffer from poor energy density and cycling life compared to top grade LIBs. One method to combat these limitations is cathode material doping.

Layered transition metal oxides (LTMO) are one of the promising cathode materials, and even though they possess several advantages, such as high specific capacities for SIBs, easy synthesis, and many modification options, they are vulnerable to Jahn-Teller distortions, chemical reactions with ambient air, and issues with the cathode-electrolyte interface.

One strategy to combat these issues is to dope the sodium sites with the intention of creating fixed ”pillars” into the sodium layers, stabilizing the crystal structure and enhancing sodium kinetics. Defect engineering via sodium and oxygen vacancies has also been shown to increase electrochemical performance, helping redox processes and shifting the crystal structure to facilitate improved sodium movement.

We carry out density functional theory (DFT) calculations of P2-Na0.67 Mn0.5 Fe0.5 O2 LTMO cathode material. Mg ions are substituted into sodium sites in both ferro- and antiferromagnetic systems and different Fe-Mn arrangements and defects are introduced to gain insights into the enhancements they bring to electrochemical properties.

We found that Mg doping improves charge movement and affects the oxidation states of the transition metals, which have a direct effect on Jahn-Teller distortions. Energy calculations reveal the feasibility of each setup as a cathode material. Defect engineering further enhances the electron conductivity and introduces new electron states near Fermi energy.

Zwitterionic Monomer as Sacrificial additive for Constructing In-Situ Polymerized Interphases in 4.8V High-Voltage LNMO Batteries

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$LiNi_{0.5}Mn_{1.5}O_4$ (LNMO) is a premier cathode candidate for next-generation lithium-ion batteries due to its high operating voltage and cobalt-free composition, which offers significant advantages in terms of cost-effectiveness and environmental sustainability.[1] However, its commercial viability is severely compromised by rapid capacity fading, stemming from the electrochemical instability of conventional electrolytes at high potentials. This degradation is particularly pronounced under constant-current constant-voltage (CCCV) cycling—the standard protocol for EVs and consumer electronics. The prolonged exposure to high potentials accelerates electrolyte decomposition and HF generation, leading to the acidic etching of the cathode surface and subsequent transition metal dissolution.[2]

In this work, we demonstrate a synergistic additive strategy employing [2-(Methacryloyloxy)ethyl]dimethyl-(3-sulfopropyl) ammonium hydroxide as a sacrificial zwitterionic monomer (1.0 wt%) combined with trimethylsilyl polyphosphate (1.0 wt%) in a commercial LP57 electrolyte. This combination facilitates the construction of a robust, in situ polymerized interfacial layer that effectively passivates the LNMO surface. Consequently, the LNMO||graphite full cell exhibits significantly enhanced durability; capacity retention improved from 70.31% to 82.96% after 200 cycles under stringent CCCV conditions (0.5C/4.8V/0.2C). This enhancement was also validated under a more aggressive low-rate CCCV mode (0.1C/4.8V/0.03C), where capacity retention increased from 83.25% to 93.72% after 35 cycles. The potent stabilization provided by the zwitterionic additive strategy offers a promising pathway for the practical market application of high-voltage LNMO-based batteries.

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Structure-function relationships of mixed Li/K highly concentrated electrolytes

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Lithium-ion batteries (LIBs) offer high energy density, long cycle life, and fast charging. Hybrid batteries using mixed-cation electrolytes incorporating charge carriers such as Li^+ and K^+ have emerged as an alternative to single-cation systems, improving ion transport, interfacial stability, and electrochemical performance.

Highly concentrated electrolytes (HCEs) enhance ionic conductivity and thermal stability through correlated ion transport via contact ion pairs and ionic aggregates, leaving little free solvent [1]. Moreover, the solid electrolyte interphase (SEI) forms primarily from anionic species, promoting cycling stability and reducing electrolyte degradation [2].

Combining mixed-cation electrolytes with HCEs offers promising synergies. Li^+ and K^+ together promote a dense, inorganic, anion-derived SEI. With graphite anodes, Li^+ provides high capacity while K^+ contributes faster dynamics for improved rate capability [3].

As proof-of-concept, we studied an HCE of 2.5 M KFSI + 2.5 M LiFSI in PC in Li || graphite half-cells, correlating HCE composition with battery performance. Results demonstrate improved rate capability and cycling stability versus single-cation HCEs. EIS reveals lower charge transfer resistance; Raman spectroscopy confirms higher ion pairing and aggregation. Elevated glass transition (Tg) and decomposition onset temperatures indicate strong ion–solvent coordination. XPS of cycled electrodes shows an SEI enriched in LiF and KF.

Future work will optimize Li/K HCE formulations to advance hybrid battery design.

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Effect of fluoride doping on electrochemical performance of regenerated Ni-Rich Li[Ni0.88Co0.09Mn0.03]O2 cathodes in lithium-ion batteries

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Ni-rich $Li[Ni_{0.88}Co_{0.09}Mn_{0.03}]O_2$ (NCM88) cathodes are interesting prospects for high-energy lithium-ion batteries, but their low cycle stability remains a serious barrier. In this work, regenerated NCM88 cathodes were manufactured utilizing a co-precipitation technique with fresh and mixed fresh-recycled metal sulfate solutions. Fluoride doping was introduced by introducing NaF at regulated quantities to assess its effect on structural and electrochemical characteristics. ICP-OES, XRD, SEM/EPMA, and XPS were used to investigate the materials' composition, structure, morphology, and surface chemistry. Coin cells' electrochemical performance was evaluated using galvanostatic charge-discharge cycling.

The findings reveal that whereas fluoride inclusion has no major effect on the layered structure, it has a considerable impact on electrochemical performance. Higher fluoride levels increase initial capacity but accelerate performance decline throughout cycling. Lower fluoride doping, on the other hand, improves capacity retention and overall cycle stability while resulting in somewhat lower starting capacity. This trend applies to materials manufactured from both fresh and recycled predecessors, emphasizing the importance of controlled fluoride content. Overall, low-level fluoride doping provides a better mix of capacity and long-term stability.

These findings offer a practical strategy to increase the endurance of regenerated Ni-rich cathodes and enabling the development of more environmentally friendly lithium-ion battery materials.

Composites of lignin-containing cellulose nanofibrils and poly (3,4-ethylenedioxythiophene) (PEDOT) for sustainable conductive material applications

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The growing interest in bio-based alternatives to conventional synthetic components of battery materials is driving force behind this work. Cellulose nanofibrils (CNF) exhibit exceptional mechanical properties with opportunity for tunable surface chemistry, making them useful for functional material development. This study focuses on chemical polymerization of 3,4-ethylenedioxythiophene (EDOT) onto lignin-containing cellulose nanofibrils (LCNF) to develop conductive composites. The longer polymer chains of PEDOT facilitated by nanostructure of cellulose fibrils resulted in development of conductive pathways. This composite binder facilitates electrode activity by not only providing mechanical stability but also improved overall conductivity. LCNF substrates with varying lignin content is used for composite preparation. Lignin is naturally occurring aromatic polymer. It is hypothesized to improve interfacial interactions with conjugated PEDOT backbone to enhance charge transport pathways in nanofibril network. Additionally, introduction of surface charge on fibrils by sulfonation(S-) is investigated. Sulfonation introduces anionic functional groups onto fiber surface. The effect of increasing ratio of conducting polymer to cellulose nanofibrils is also investigated. The prepared films of PEDOT-coated LCNF and S-LCNF are characterized for electrical conductivity, surface morphology and chemical composition. Lignin content is found to influence PEDOT polymerization and film conductivity and fiber surface sulfonation affects uniform PEDOT chains deposition. Overall, this work demonstrates LCNF as suitable platform for binder applications. Tuning lignin content and introducing surface charge on fibrils represent effective strategies for optimizing surface coating of fibrils with conducting polymers. This study is indicative for next-stage deployment of this type of bio-based materials for applications as sustainable electrode materials.

Membranes containing cyclic ammoniums as ion exchange groups for all-vanadium flow batteries: A comparative study

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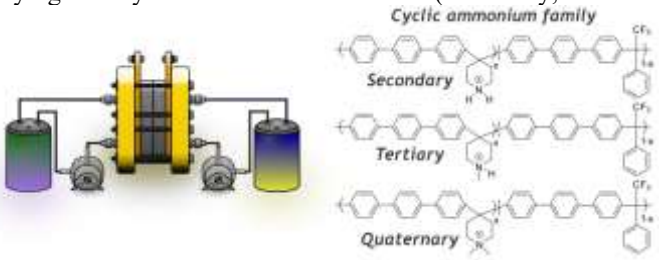
The all-vanadium flow battery (VFB) has proven to be a promising technology for achieving grid stability while being a safer option compared to lithium-ion batteries. One major challenge with VFBs is the electrolyte crossover. Using the benchmark membrane Nafion is associated with high cost, accounting for about one third of the cost of a VFB stack [1] and can result in a significant crossover of species through the membrane. One strategy to minimize electrolyte crossover is using anion exchange membranes, which exclude vanadium ions due to the Donnan exclusion effect. Novel non-fluorinated anion exchange membranes have recently received a lot of attention for VFBs [2-4]. Poly(arylene peridinium)-based anion exchange membranes (PAP) have proven high performance in VFBs, as previously reported by our research group. In several aspects, these membranes not only have superior performance compared to Nafion 212, but are also chemically stable in highly acidic media up to over 800 hours [1].anion exchange membranes carrying cyclic ammoniums (secondary, tertiary and quaternary) groups



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Synthesis and electrochemical properties of LiMn1-xFexPO4 for lithium-ion batteries

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Lithium-ion batteries remain a cornerstone of modern energy storage technologies, powering applications from portable electronics to electric vehicles. Lithium iron phosphate is one of the most widely used lithium-ion battery materials, however, due to its low voltage plateau, other options need to be studied in order to meet the demands of high energy density batteries. Although lithium manganese phosphate demonstrates higher energy density, it shows inferior rate capabilities due to lower electronic conductivity. Combining the high stability of LiFePO4 and high energy density of LiMnPO4, LiMn1-xFexPO4 could be a promising cathode material for lithium-ion batteries.
In this work LiMn1-xFePO4 was synthesized using different methods and obtained powders were analysed using XRD, SEM and ICP-MS to confirm the desired composition and morphology. Electrochemical properties were determined using galvanostatic charge-discharge measurements and electrode composition was optimized.
Based on the results conclusions were drawn about the optimal method of synthesis and electrode composition. The findings contribute to the development of optimized LiMnFePO4 systems for high-performance next-generation batteries.

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Interfacial Engineering for Enhanced Performance of Aqueous Zinc-Ion Battery

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In recent years, aqueous zinc ion batteries (AZIBs) have attracted significant attention in energy storage due to their notable advantages, including high safety, low cost, high capacity, and environmental benignity. However, the critical challenges related to the electrode-electrolyte interfaces cause problems to both anode and cathode, including uncontrolled side reactions, dendrite formation, and active materials dissolution. This limits their cycling performance and implementation in real applications. Development of efficient interfacial engineering strategies that can simultaneously address issues on both cathode and anode is highly desirable and strategically important for the full cell. In this work, we have developed a versatile interfacial modification approach, which allows formation of a thin and controllable protective coating on both cathode and anode in AZIBs. The established network reduces active water activities, suppress parasitic side-reactions, and promotes uniform zinc deposition on zinc anode. Application on MnO2 cathode enhanced rate capability, improved storage capacity, and strengthened structural stability during cycling. The dual-electrode modification demonstrated substantially improved specific capacity, enhanced rate capability, and superior cycling stability compared to unmodified systems. This study provides a facile and scalable approach to address multiple interfacial challenges in aqueous battery systems simultaneously.

Leveraging black liquor inorganics to catalytically crosslink kraft lignin and produce morphology defined hard carbons

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Conventional routes for converting kraft lignin (KL) into hard carbons typically rely on highly purified (low-ash) feedstocks and slow, energy-intensive oxidative stabilization steps which are often assisted by added crosslinkers to mitigate melting and foaming during thermal treatment. In this work, we deliberately invert this paradigm by exploiting, rather than removing, pulping-derived inorganic species as intrinsic catalysts for lignin stabilization.

Spherical KL microparticles (KL-MP) were recovered from softwood black liquor using alternative membrane or CO2-assisted precipitation technologies, intentionally retaining inorganic sodium (Na) salts and organically bound Na species. These materials were compared with an acid-precipitated, low-ash reference KL (KL-REF). During thermal pretreatment in air, KL-MP undergoes rapid inorganic-catalysed oxidative crosslinking which suppressed melting, foaming, and particle fusion. In contrast, KL-REF softens and foams under identical conditions. Following pretreatment, inorganics are removed by washing and the stabilized KL-MP is carbonized, yielding low-surface-area hard carbons that preserve the original micron-scale spherical morphology. Removal of the catalysing inorganics after the oxidative crosslinking allows their recirculation back to main pulping process. When evaluated as Li-ion battery anodes, the resulting hard carbons exhibit improved electrochemical performance compared to carbons derived from KL-REF. Overall, this study demonstrates how typically undesirable inorganic impurities can be leveraged to simplify lignin thermal conversion, offering a scalable route to morphology-controlled carbon materials for energy storage and other applications for which particle size and morphology are critical.

Crucial impact of salt and additives in polymer electrolytes for low-temperature operation solid-state Na batteries

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Crucial impact of salt and additives in polymer electrolytes for low-temperature operation solid-state Na batteries

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Rechargeable solid-state sodium batteries are promising candidates for next-generation high energy storage systems. Sodium is abundant and cost-effective compared to lithium, and its use with solid electrolytes can address safety concerns associated with metal anode batteries (Li, Na) using liquid aprotic electrolytes. Polymeric solid electrolytes offer flexibility and good interfacial contact without external pressure; however, they suffer from low room temperature ionic conductivity and high interfacial resistance.

Na||NVP solid-state cells are demonstrated using composite polymer electrolytes based on PEO with sodium salts (NaFSI and NaTFSI), with small amounts of ceramic additives[1]. Optimized electrolytes were developed and systematically studied. Ceramic additives enhance Na^+ ionic conductivity, salt dissociation, electrochemical stability window, and electrode–electrolyte interfacial properties[2]. Consequently, Na||NVP cells exhibit stable high rate performance (1C) at 40 °C over hundreds of cycles, delivering capacities above 80 mAh g^{-1} with near 100% Coulombic efficiency and excellent retention. These improvements demonstrate the synergistic effect of salt chemistry and ceramic additives in tuning electrolyte performance. The role of each component in bulk and interfacial behavior is analyzed.

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Facet-controlled synthesis of spinel LiMn2O4 as cathode material for Li-ion batteries

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The development of sustainable battery chemistries and reducing dependence on critical minerals underline the need for cobalt-free cathodes. Spinel-type $LiMn_2O_4$ (LMO) is a popular choice for this application. However, it is imperative to further improve its capacity retention and cyclability to widen its commercial application. Mn-dissolution is one of the major factors that limit the performance of LMO. It causes capacity fade, especially at elevated temperatures and potentials (>4.1V vs Li/Li+)[1]. Particle morphology and crystal facets play a crucial role in determining the performance of the material[2]. Depending on the crystal facets exposed, the extent of Mn dissolution can be reduced. Moreover, the facet exposure also affects the quality of cathode-electrolyte-interface (CEI) that inherently forms during the initial formation cycles.

To study these effects, we first synthesize LMO particles with great facet control and material purity, thus enabling particles with only the desired facet exposed. This study investigates the effect of synthesis parameters such as lithium salt, calcination temperature, time and reaction environment towards achieving control on facet exposure. XRD and SEM of the samples across a wide parameter matrix provide the insights needed to design the synthesis protocol for the desired LMO facet exposure. Electrochemical testing in a half-cell format helps in understanding the role of facet control in the performance of the cathode material. This work helps to develop LMO required for further studying Mn-dissolution and facet-dependent CEI formation.

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Fluorine-Free Sweet Ionic Liquids and Electrolytes

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We have developed fluorine-free and flame-resistant electrolytes based on ionic liquids (ILs) comprising the non-nutritive sweetener, saccharinate (Sac) anion, coupled to a wide range of organic cations [1-3]. These ILs exhibit beneficial thermal, physicochemical and electrochemical properties. By IR spectroscopy we find the ionic interactions to be controlled by the distinct conformers of the Sac anion, which in turn are cation dependent. Among the ILs, (P4444)(Sac) showed the lowest glass transition temperature, the highest thermal stability and ionic conductivity, and the widest electrochemical stability window, up to 6 V. Used as an electrolyte in a symmetric supercapacitor, it enabled a specific capacitance of 204 F g-1 at 1 mV s-1, an energy density of 53 Wh kg□1 and a power density of 300 W kg-1 at a current density of 0.1 A g-1, and the supercapacitor retained 81% of its initial capacitance after 10000 cycles at 60 ºC. Furthermore, creating dual-salt battery electrolytes based on combining the LiSac and lithium bis(oxalato)borate (LiBOB) salts in triethyl phosphate (TEP) as single solvent, with vinylene carbonate (VC) as additive, enabled stable cycling and a capacity retention of 86% in both Li//LFP and Li//NMC811 cells after 500 cycles at 1C rate – hence offering an intrinsically safer electrolyte that also enables the use of both lithium metal anodes and medium-to-high-voltage cathodes.

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Synthesis of lithium-rich cobalt-free layered oxide cathode material $Li_{1.16}Ni_{0.19}Fe_{0.18}Mn_{0.46}O_2$ and its electrochemical properties

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Lithium-rich layered oxides are an attractive class of cathode materials for lithium-ion batteries due to their high specific capacities (>250 mAh/g). However, their practical application is limited by capacity and voltage fade, caused by structural modifications during cycling. Furthermore, many high-performance layered oxides include scarcely available cobalt, motivating the development of cobalt-free alternatives with improved structural stability.
In this study, a cobalt-free lithium-rich cathode material $Li_{1.16}Ni_{0.19}Fe_{0.18}Mn_{0.46}O_2$ was synthesized via a hydroxide co-precipitation method followed by solid-state calcination and high-temperature sintering. The effect of sintering temperature and lithium excess on phase composition and electrochemical performance was investigated. X-ray diffraction analysis confirms the coexistence of a layered α-$NaFeO_2$ - type phase and a monoclinic Li_2MnO_3 phase, with their relative proportions strongly dependent on sintering conditions.
Galvanostatic charge-discharge measurements show that the sample synthesized at 750 ^oC with 10% excess lithium exhibits the best performance, delivering an initial discharge capacity of 200 mAh/g at 0.1 C and 150 mAh/g at 0.2 C. Despite forming the expected lithium-rich structure, the capacity remains below typical values reported for lithium-rich materials, which is attributed to increased charge transfer resistance, as indicated by electrochemical impedance spectroscopy.
These results emphasize the strong dependence of electrochemical performance on synthesis conditions and underline the importance of optimizing lithium content and thermal treatment to improve the performance of cobalt-free lithium-rich cathodes.

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Conversion of kraft-lignin into battery grade graphite using spray-pyrolysis–derived catalysts with tuned properties

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The development of sustainable alternatives to fossil-based graphite is essential for lithium-ion battery technologies. Kraft lignin, an abundant by-product of the pulp and paper industry, is a promising renewable precursor due to its high carbon content and aromatic structure. However, its graphitization remains challenging because of its complex and disordered structure. Catalytic graphitization is an effective approach to address this, where catalyst size, morphology, and structure play key roles.

In this work, Fe–Zn bimetallic catalysts are produced via a novel ultrasonic spray drying approach using different Fe:Zn ratios (2:1, 3:1, and 4:1). This method enables the formation of spherical catalyst particles with an average size of ~15 µm and controlled morphology. A uniform distribution of iron and zinc within the particles is confirmed by energy-dispersive spectroscopy (EDS), highlighting the effectiveness of the synthesis strategy.

The catalyst–lignin composites are subjected to carbonization followed by high-temperature graphitization (up to ~2400 °C under inert atmosphere). The effect of Fe:Zn ratio on graphitization is systematically evaluated using X-ray diffraction, Raman spectroscopy, and electron microscopy (SEM and TEM). The results show that catalyst composition strongly influences the degree of graphitization and the resulting carbon structure.

Electrochemical measurements are conducted to evaluate the performance of synthesized carbon materials as anodes in lithium-ion battery half-cells. Results are compared across catalysts with different Fe:Zn ratios, revealing the influence of catalyst composition on electrochemical behavior. These findings demonstrate the potential of spray drying controlled catalyst design for sustainable carbon materials for energy storage applications.

Battery-Grade Hard Carbon for Na-ion Batteries

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Compared to its well spread Li-ion batteries (LIBs) predecessor, Na-ion batteries (NIBs) technology offers a potentially more environmentally friendly alternative with some performance advantages. Cost-effectiveness, safety, balance of power and energy density make NIBs as a preferable option for use in large-scale energy storage systems. Currently, the research in the field of NIBs is mainly focused on active materials with the aim of improving performance characteristics. Among many materials used for NIBs anodes, hard carbon (HC) materials are the most popular choice for commercial batteries or prototypes. However, the choice of precursors severely affects the electrochemical performance of these materials, making direct preparation of HC with programmed properties almost impossible.

In this study, a comprehensive evaluation of potential precursors for HC anodes that are accessible in Norway will be beneficial to the greater scientific community. The application of a wide variety of characterization techniques for the different HC materials will help reinforce the basic understanding by deepening the comprehension of the basic relationships between the precursor, processing into HC, and final cell characterizations. It will be possible to fully correlate structural features with electrochemistry through operando characterization.

The selection of the precursors for the project was driven by their scalability and local availability: they come from domestic sources, including industrial carbon provided by the industry partners and forestry waste. The main outcome of the proposed research is the development of low-cost battery-grade HCs with low environmental impact, stable and predictable electrochemical performance.

Synthesis of Catalyst-driven Sustainable Hard Carbon via Defect Engineering for Sodium−Ion Batteries

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Biomass-derived hard carbon has emerged as a sustainable and tunable anode material for sodium-ion batteries due to its adaptable defect chemistry, interlayer spacing, and disordered carbon framework. Herein, coconut-shell-derived hard carbon was engineered through chemical activation, heteroatom treatment, transition-metal incorporation (Fe, Ni, Mn and Co), and a ZIF-derived precursor strategy to investigate catalyst-driven structural evolution during carbonization. A series of catalyst-engineered hard carbons was synthesized through controlled pyrolysis and characterized using X-ray diffraction, Raman spectroscopy, scanning electron microscopy, and energy dispersive spectroscopy. Structural analysis revealed catalyst-dependent evolution of disorder, interlayer spacing, graphitic domains, and localized carbon reconstruction. Potassium hydroxide activation moderately improved short-range ordering, reducing the Raman ID/IG ratio from 0.98 to 0.91. Nitrogen doping shifted the broad carbon reflection from ~26.6º to 25.8º, indicating expanded turbostratic carbon layer spacing beneficial for sodium-ion diffusion. Transition-metal incorporation further induced localized graphitization and defect generation through catalyst-assisted carbon restructuring. Ni-modified hard carbon exhibited enhanced graphitic ordering with graphitic domain size of ~ 9 nm, suggesting catalytic promotion of sp2-rich carbon domains and improved structural connectively. Raman analysis further demonstrated evolution of defect-related carbon features across the sample series, with metal-modified carbon exhibiting pronounced lattice distortion and localized metal-carbon interactions. The ZIF-derived system produced partially graphitized yet defect-rich porous carbon architectures without conventional chemical activation, highlighting an alternative pathway for microstructural tuning. This study provides mechanistic insights into catalyst-mediated defect engineering in sustainable hard carbon systems and highlights the potential of biomass-derived carbon architectures as tunable anodes materials for advanced sodium-ion battery applications.

Off-stoichiometry in Na2.43Fe1.24(SO4)3 cathode and Insights into phase evolution and high-voltage stability for sodium-ion batteries

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Lithium ion batteries have been the mainstay of the portable electronics industry for decades. However the resource scarcity and the geopolitical tensions necessitate diversification of the rechargeable battery chemistries for efficient management of renewable energy sources and hence to limit the fossil fuel reliance. Sodium ion batteries are known to be a viable alternative; however, the practical implementations are largely limited by poor intercalation kinetics and electrode instabilities of the positive electrodes at the higher voltage operations. Na-Fe-SO4 ternary system forms several earth abundant inexpensive cathodes with varying elemental combinations. These materials exhibit higher operating voltage (~3.8 V vs Na) attributable to the Fe3+/Fe2+ redox potential and robust architecture relaying on stable SO4 polyanionic network. This work details the synthesis, electrochemical properties and structural changes happening during the Na-ion de/intercalation to the Na2.43Fe1.24(SO4)3 cathode. In addition to the standard alluaudite phase as primary phase, traces of Na6Fe(SO4)4 and/or little amorphicity is also been identified. The heterogeneous nature facilitates stable electrochemical characteristics closely aligned with thermotical capacities over extended cycles with excellent capacity retentions. The structural changes happening during ion movement is investigated in detail with ex-situ and operando techniques. In departure from the several of the existing reports, the study points probable additional phase formations along side the total crystallinity drop during the Na-ion removal from the structure.

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 (LIBs) 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.

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. 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 these polymers in Si anodes for LIBs.

Self-healing properties of polymers are typically evaluated in pure polymer films. A micro sized cut is made and one studies the ability to repair this cut upon heating. The presence of other materials in the polymer film affects the healing properties (see figure). In batteries, the polymer additive is only a small fraction of the electrode (<10 wt%), which completely changes the playing field to test self-healing capabilities. A common understanding on testing self-healing mechanisms in batteries will help to advance the integration of materials with smart functionalities in batteries. Hence, a testing matrix is needed to bridge the gap between polymer model systems and functional battery electrodes. This contribution conference will focus on the advancements and challenges encountered while working towards this goal.

Effects of chemical prelithiation of Silicon nanopowder for Lithium-Ion Battery Anodes

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Continuous improvement of lithium-ion batteries is integral for advances in modern technology and for reaching the goals set by the United Nations. While commercial lithium-ion batteries are based on graphite negative electrodes with a specific capacity of 372 mAh g-1, silicon-based negative electrodes possess a theoretical specific capacity of 3579 mAh g-1, while maintaining a suitable discharge voltage of ca. 0.4 V, being abundant, non-toxic, and environmentally benign. Aside from these advantages, silicon-based negative electrodes show poor capacity retention, cracking due to large volume expansion, and an unstable solid-electrolyte interphase (SEI). A prelithiation can lead to a more controlled SEI formation in the formation cycles and increase the Initial coulombic efficiency, resulting in better capacity retention[1].

The chemical prelithiation of silicon nanopowder prior to electrode fabrication will be investigated in this work. Unlike conventional electrode level prelithiation, this enables the formation of the binder and conductive network around already partially expanded silicon nanoparticles, reducing mechanical degradation and contributing to increased capacity retention. Additionally, no binder compatibility challenges arise in this process. In this work electrodes consisting of prelithiated, and non-prelithiated silicon nanopowder are fabricated for electrochemical testing in half-cell configuration. Additionally, dilatometry is employed to observe the dilation and contraction of the electrode during cycling.

This study systematically investigates the performance-enhancing mechanisms of powder prelithiation for silicon-based negative electrodes in lithium-ion batteries.

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Zn based MOF-Celgard composite membranes for enhanced selectivity in nonaqueous redox flow batteries

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Keywords: redox flow battery, metal-organic framework, ion selectivity, composite membrane
Background

Nonaqueous redox flow batteries (NARFBs) have attracted increasing attention for grid-scale energy storage due to their wide electrochemical window and high theoretical energy density. However, their practical application has been limited by the lack of membranes with high ionic conductivity and effective suppression of active species crossover in organic electrolytes.
Results

In this study, a composite membrane was fabricated by electrodepositing a metal–organic framework (MOF) layer onto a commercial Celgard separator. The electrodeposition process enabled uniform and controllable MOF growth on the porous substrate, provided ordered nanochannels that regulated ion transport pathways within the separator. The obtained membrane was further evaluated its selectivity and performance in a lithium/FcTFSI based NARFB system, consisting of a ternary organic mixture (EC/PC/EMC) with LiTFSI as the supporting electrolyte, with particular emphasis on the selective permeation of LiTFSI and FcTFSI. The results indicated that MOF-modified membranes facilitated the transport of LiTFSI while effectively hindering the crossover of FcTFSI. Electrochemical characterization further showed that the composite membranes exhibited enhanced ion selectivity while maintaining comparable ionic conductivity. Such selective ion transport contributed to improved operational stability and extended battery lifetime.
Conclusions

This work demonstrates that MOF-modified composite membranes can effectively increase selective transport in nonaqueous electrolyte systems. In the solution , the membrane exhibited preferential permeation of LiTFSI while suppressing FcTFSI crossover, thereby enhancing ion selectivity without sacrificing ionic conductivity. These findings provide a promising pathway for developing high-selective separators for nonaqueous redox flow batteries.

Synthesis of $LiFePO_4$ Cathode Materials via Recovery of Iron and Phosphorus containing Industry Waste.

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Significant attention has focused on olivine-structured $LiFePO_4$ (LFP) as a promising cathode active material for lithium-ion batteries due to its thermal stability, long cycle life, and cost-effectiveness. However, challenges related to precursor purity, resource sustainability, and increasing industrial waste streams necessitate alternative synthesis strategies that are both efficient and circular.

In this study, an Fe- and P-containing industrial side stream was utilised as a precursor for LFP synthesis through a selective leaching and phase transformation approach. Acid leaching under strongly acidic conditions (pH < 2) using varying HCl concentrations enabled the removal of Ca- and Mg-containing phases while retaining Fe–P-rich solids. The resulting residue was hydrothermally treated to produce $FePO_4$ as the dominant phase, alongside minor magnetite (Fe_3O_4). This $FePO_4$ was subsequently employed as a precursor for LFP synthesis via a solid-state lithiation route, demonstrating the feasibility of converting industrial waste into functional battery materials.

In parallel, LFP was synthesised from virgin precursors using hydrothermal and solvothermal methods to establish a performance benchmark. These routes yielded phase-pure LFP with particle sizes ranging from approximately 200 nm to 1 µm, enabling comparison with materials derived from side streams.

The combined approach highlights the potential of integrating recycled and conventional synthesis pathways, where controlled impurity retention and particle-size variability may enable defect-engineered, high-performance LFP. This work contributes to the development of scalable, resource-efficient, and sustainable battery material production strategies.

Enhancing structural and electrochemical stability of NMC955 cathodes by W/B core-shell co-doping via microwave-assisted synthesis

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Lithium-ion batteries (LIBs) remain the leading energy storage technology owing to their high energy density, long cycle life, and high efficiency. Ni-rich layered oxides such as $LiNi_{0.90}Mn_{0.05}Co_{0.05}O_2$ (NMC955) are promising cathode materials because of their high specific capacity and reduced cobalt content. However, their practical application is limited by surface degradation, lattice instability, transition-metal migration, and rapid capacity fading during high-voltage cycling.
Herein, a microwave-assisted core–shell W/B co-doping strategy was developed to enhance the structural and electrochemical stability of NMC955 cathodes. W and B were selected as complementary dopants: W strengthens the bulk lattice through strong W–O bonding and helps suppress Li^+/Ni^{2+} cation mixing, while B improves surface stability, reinforces the oxygen framework, and reduces parasitic interfacial reactions. Precursor materials were synthesized by a microwave-assisted hydrothermal method, enabling rapid reaction within 30 min, uniform heating, and controlled particle morphology. Core dopants were introduced during precursor synthesis, whereas shell dopants were incorporated during lithiation step (Fig.1). This approach enabled the preparation of nine samples, including undoped, single-site doped, and dual-site co-doped NMC955 materials. Among all samples, LNMC-W(core)-B(shell) delivered the best performance, achieving an initial discharge capacity of 226 mAh g^{-1} at 0.1C and 88% capacity retention after 100 cycles at 0.5C, compared with 75% for undoped LNMC-0-0. Differential capacity analysis confirmed reduced polarization and stabilized phase transitions, demonstrating that W/B core–shell co-doping effectively improves the durability of Ni-rich cathodes. Overall, this work highlights microwave-assisted W/B co-doping as a scalable strategy for designing durable, high-capacity Ni-rich cathodes for next-generation LIBs.

Modelling ionic liquid (electrolyte) conductivity using symbolic regression

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The high thermal stabilities, wide electrochemical stability windows, and inherently good ionic conductivities of ionic liquids (ILs) make them promising alternatives to conventional solvents in battery electrolytes [1]. However, many properties of IL based electrolytes remain poorly understood, particularly the underlying factors that govern ion transport.

As ILs constitute a vast chemical space, which could exceed 10^18 unique compositions [2], modelling, and especially machine learning (ML) approaches, offers an efficient route to assess their properties. Conventional ML methods, however, lack interpretability. To better understand ion transport in neat ILs, we have recently explored symbolic regression (SR), an ML method that finds analytical equations [3]. By using a general equation derived from free volume theory (FVT) as a template, we let SR find analytical models consistent with an ion-hopping mechanism. Using molecular descriptors as inputs, we considered over 300 ILs and found models capturing ionic conductivity across wide temperature ranges.

We are now extending our SR-approach to IL-based battery electrolytes, i.e. ILs doped with Li-, Na-, or K-salts. We are especially interested in trying to model the transport of the alkali cations, gaining molecular insights in how to design IL-based electrolytes with high cation transport numbers. One direction we are currently exploring is to combine SR with physics-informed neural networks (PINNs), which could help us extend existing theoretical frameworks with novel insights.

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Reproducible benchmarking of battery equivalent circuit model parameter estimation

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Background
Accurate parameter identification is essential for the reliable use of equivalent circuit battery models in battery management systems. However, comparing estimation methods remains difficult because reported studies often differ in experimental protocols, SOC and OCV handling, sampling rates, noise levels, and software implementation details.

Results
This work presents a reproducible benchmarking framework for evaluating parameter estimation algorithms for battery equivalent circuit models under controlled and transparent conditions. Synthetic measurement sets are generated from charge and discharge operating profiles and augmented with configurable perturbations, including sensor noise, different data-logging frequencies, and systematic OCV model mismatch. By keeping the data generation process, model structure, and evaluation metrics fixed, the framework isolates the effect of the estimation algorithm itself. The initial implementation focuses on a family of least squares based estimators and compares their behaviour in terms of voltage prediction error, convergence robustness, computational cost, and sensitivity to imperfect input information.

Conclusions
The proposed framework provides a neutral basis for fair comparison of battery model parameterisation methods and reduces dependence on proprietary or insufficiently documented toolboxes. It supports reproducible assessment of estimator performance under realistic error sources and can be extended to additional model structures, ageing conditions, temperatures, and dynamic load profiles. This contributes towards more transparent development of battery models for monitoring, control, and digital twin applications.

Development of AI-Based Data-Driven Aging Model for Li-Ion Batteries

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With the increasing use of lithium batteries, especially in battery storage systems (BESS), accurately predicting their remaining lifespan has become an important research topic in the energy sector. Compared to traditional batteries, lithium batteries face more complex usage scenarios, especially under varying conditions during charging and discharging, which require prediction models with greater generality and accuracy. In recent years, some studies have introduced neural networks into lithium battery prediction to more accurately simulate their charging and discharging behavior and characteristics. Machine learning methods, including MLPs and LSTM, have made initial progress in predicting two key parameters of lithium battery lifespan: SOH and RUL.
However, due to inherent limitations, existing models still have shortcomings in general- ization ability and decision accuracy.
To address these issues, this study proposes a neural network-based Transformer model. Model variants were constructed by adjusting different hyperparameter combinations, and the performance of selected models was evaluated based on MAE and RMSE on a validation set. The Transformer model is compared with MLP and LSTM models, and their performance is discussed.
The results show that the Transformer-based model significantly outperforms MLPs and LSTM models in both the overall and subgroup tests, validating the effectiveness of the proposed method. In summary, this study provides a new approach to Transformer modeling for lithium-ion battery BESS applications and compares the application potential of different modeling methods.

Electrode-electrolyte interfaces of chloroaluminate ionic liquids with and without solvents by constant potential molecular simulations

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Aluminium-carbon batteries are promising next-generation secondary batteries with high power density that can potentially be manufactured much cheaper than Li-ion batteries. The first reported ionic liquid electrolyte is still the state-of-the art; AlCl3-[EMIm]Cl, which contains EMIm+, Al2Cl7- and AlCl4- ionic species, of which the two latter are active in the anode and cathode half reactions, respectively. However, the interfacial properties of the ionic liquid electrolyte against the Al anode and graphite cathode are still poorly understood.

In this work, we present a modeling study of the interfaces composed of Al electrodes and the ionic liquid, including the electric double layer (EDL) formed at the interface. We utilize constant potential molecular dynamics simulations to model the electrified interface for different potential differences across the cell and different electrolyte compositions. We analyze the density profile of electrolyte species in the interface and find that the presence of only charged species causes charge overscreening and ionic layering extending far into the electrolyte. The ionic species are highly oriented in the interface region next to the electrode, increasing the packing density. The residence time of the species is about an order of magnitude higher in the interfaces compared to the bulk phase, indicating that the interface constitutes a considerable barrier against ion transport.

We examine the influence of adding neutral solvent species to the electrolyte; tetraglyme or monoglyme, both in the bulk phase and in the interfaces. The influence on the structure and transport properties of the bulk electrolyte and the interfaces are studied.

A flow battery model for overpotential distribution and optimal cell design

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Background

Flow batteries are often presented as a promising candidate for low-cost stationary energy storage. They are commonly based on aqueous catholyte and anolyte, where dissolved redox-active species with different redox potentials store energy. The best-known type depends on vanadium, but all sorts of redox-active and soluble species could be used to make redox flow batteries in principle. However, the optimal cell design depends strongly on what redox species are chosen, and numerical modelling can greatly help finding the right design for the right species. The model in this work was developed as part of the EU-funded Rezilient project, where the goal is to develop a redox mediated Zn-air flow battery.

Results

A spatially resolved numerical continuum model for flow batteries is presented. It reproduces experimental current-voltage curves with high accuracy. It shows how overpotentials are distributed in the system as a function of various parameters, such as electrode thickness, electrode porosity, flow speed, mediator concentrations, mediator potentials and current density. We also present how the overpotential distribution affects the attainable efficiency of the battery.

Conclusion

Optimal flow battery cell design depends strongly on the chosen redox active species, the intended discharge rate and the sensitivity to decreased efficiency. We show that there are clear optima in design parameters such as electrode thickness and electrode porosity.

Multiscale modeling of aging mechanisms in lithium-ion batteries

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To decrease carbon emissions as part of the goal to reach net-zero emissions by 2050, transitioning to electric vehicles in the transport industry is crucial. Lithium-ion batteries are an important part of this transition as they provide high energy density and are rechargeable. However, cycling of lithium-ion batteries lead to aging due to mechanical and chemical degradation mechanisms. Electrolyte motion caused by intercalation swelling and mechanical load in the electrodes may contribute to degradation and a decrease in capacity. This phenomenon was recently highlighted by Solchenbach et al. (2024) and Bond et al. (2025). To understand this phenomenon better, it is of interest to develop models which accurately capture how the electrodes deform during cycling. In this work, the poroelastic properties of the negative and positive electrodes are evaluated using microscale simulations. The simulations are based on geometries from computed tomography scans. The porosity, permeability and stiffness of the electrode are evaluated under different state of charge and boundary conditions. The constitutive relations from the poroelastic model, which link volumetric strain and fluid motion, are calibrated using the results from the microscale simulations. The poroelastic model is then implemented in macroscale models where the aging mechanisms can be studied on the cell level. The results from the work will aid in battery design to mitigate the aging effects that are accelerated by electrolyte motion.

Enhancing lithium-ion battery state of health estimation through strain signal integration and machine learning

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Background:
Continuous, real-time monitoring of battery State of Health (SoH) is critical for safe and reliable operation. Conventional SoH estimation relies mainly on electrochemical metrics such as capacity and voltage, while temperature is typically used only as an average operating parameter. Recent studies have shown that fibre-optic temperature sensing can improve SoH assessment. Here, we investigate whether real-time strain measurements from optical fibre Bragg grating sensors can further enhance capacity fade and SoH estimation using previously collected cycling data from commercial cells(Ghashghaie et al., 2024).
Results:
A gradient-boosted decision tree (XGBoost) regressor was used to compare three models: all features, electrochemical-only, and strain-only. Combining strain and electrochemical features improved predictive performance, increasing R^2 from 0.993 to 0.996 and reducing RMSE from 0.400 to 0.295. Feature importance analysis identified strain-derived variables as major contributors. Five-fold cross-validation also showed lower RMSE when strain data were included (0.171 vs 0.234). The combined-feature model achieved an R^2 of 0.996 for SoH estimation. A further validation model using cells from two chemistries produced an R^2 of 0.945.
Conclusions:
Mechanical strain is a valuable diagnostic signal for battery degradation and significantly improves SoH prediction when integrated with electrochemical data. These findings demonstrate the potential of real-time, non-invasive fibre-optic strain sensing for scalable, interpretable, and sensor-agnostic battery health monitoring frameworks.
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Parameter sensitivity and parameter identification of Electrochemical-Thermal models under different operating conditions

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The shift towards electrification highlights the essential role of Lithium-ion batteries (LIBs) and accurate prediction of battery performance. Physics Based Modeling (PBM) proposed a reliable method for understanding the internal states of the batteries, however, it raises challenges due to the complexity of Electrochemical-thermal models and absence of a single universally accepted approach for parametrization of such models. In this work, a Pseudo-2-Dimensional (P2D) model is developed for Li-ion battery performance through different operating conditions to evaluate the prediction accuracy of LIB P2D models. A systematic classification framework of parameter obtention was also proposed through multi-steps for P2D electrochemical models along with an optimization-based calibration methodology. Furthermore, this work evaluates the continuum physics-based model incorporating various electrode-scale heat generation mechanisms to better understand how selected parameters influence the cell's electrochemical–thermal behavior under different conditions.

Analytical pulsing protocol to parametrise physics-based battery models

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Physics based battery models such as the Doyle-Fuller-Newman (DFN) model provide detailed insight into lithium ion battery behaviour but are often limited by complex and time consuming parametrisation. The recently proposed Analytical Pulsing Protocol (APP) enables extraction and decoupling of thermodynamic, kinetic, and transport information from full cell measurements without extensive equilibration. This work evaluates APP as the primary experimental basis for DFN parametrisation using minimal supplementary measurements.

APP characterisation was combined with geometric measurements, scanning electron microscopy, and literature values to construct a streamlined DFN parametrisation workflow. Electrode stoichiometric bounds were optimised against pseudo open circuit voltage data, while the most sensitive kinetic parameters were refined using particle swarm and Gaussian process based Bayesian optimisation. The resulting parameter set reproduces the main APP pulse characteristics across the state of charge range and captures dominant kinetic behaviour. Independent validation against constant current discharge tests, not used for optimisation, shows reasonable agreement across multiple C rates, although discrepancies remain for mass transport related behaviour.

The results demonstrate that APP can serve as a practical and information rich foundation for DFN parametrisation with reduced experimental effort. More importantly, APP provides a structured framework for systematic comparison of experimental and simulated responses, lowering barriers to applying physics based battery models in research and industrial applications.

Investigating diffusion mechanisms in superionic ceramic electrolytes

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Studying diffusion in solid ceramic electrolytes furthers the understanding of diffusion processes in all-solid-state batteries, with the potential to improve their performance. By harnessing the strength of different computational methods, we investigate diffusion in a range of ceramic electrolyte and electrode materials. Specifically, we investigate the impact of different configuration entropy contributions on the diffusion[1]. Most importantly, we show that explicitly time-dependent correlation effects are not necessary to explain the effective energy barriers related to ion diffusion in ceramic electrolytes. Furthermore, we apply our methods to gain a better understanding of the Li-diffusivity in the prominent LATP solid electrolyte[2]. By studying a wide range of Aluminum substitution concentrations, we identify the Li-ion concentration as the main reason for increased diffusivity, while the experimentally observed reduction of the conductivity at larger substitution concentrations can be explained by local and macroscopic structural rearrangements. Overall, we highlight the strengths and weaknesses of different computational tools and how they can aid in understanding and designing new solid ceramic electrolytes.

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A Browser-Based Virtual Battery Laboratory for Interactive Physics-Based Learning

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This work presents a browser-native virtual battery laboratory that integrates the PyBaMM electrochemical modelling framework, the Pyodide in-browser Python runtime, and the Godot engine to create an accessible, installation-free learning environment for battery education. As shown in Figure 1, the platform provides a web-based front page through which users can select among four virtual laboratories focused on cycling performance, material and geometry sensitivity, charging strategies, and electrochemical impedance spectroscopy. The system executes physics-based simulations locally on the user's device through WebAssembly and dedicated Web Workers, ensuring responsiveness, privacy, and independence from server-side infrastructure. By combining research-grade battery models with an intuitive graphical interface, the platform enables students to explore battery behaviour interactively, compare scenarios side by side, and obtain immediate visual feedback through high-quality plots. This approach addresses the major limitations of conventional battery teaching laboratories, including high equipment cost, long experiment times, and safety risks. The local-first architecture also supports offline use after caching and aligns well with modern classroom and remote-learning requirements. Overall, the results demonstrate that the integration of PyBaMM, Pyodide, and Godot provides a reliable, scalable, and pedagogically effective solution for teaching electrochemical energy storage concepts, while preserving the scientific rigour needed for meaningful experimentation and student engagement.

EnGOAT – A Tool For Studying Mass Transport in Crystaline Materials

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By connecting material structure, energy landscape, and ion transport properties, the Energy Geometry Analysis Toolkit (EnGOAT) enables detailed insight into the structure–activity relationships governing ionic conductivity in solid-state ion conductors. EnGOAT provides automated, fast, and reliable computation of host-structure energetics and geometry, while predicting ion transport properties several orders of magnitude faster than state-of-the-art molecular dynamics. The method is broadly applicable, requiring no prior knowledge of diffusion pathway topology, efficient and automatable and is thus well suited for high-throughput screening. EnGOAT generates high-quality, physically grounded data that can support the development of physics-informed machine-learning models and help guide experimental design and materials optimization. Its integrated visualization tools enable analysis of energy basins, transition states, and minimum-energy diffusion pathways, contributing to a predictive and interpretable framework for solid-state electrolyte development.

State-of-Charge Estimation Under SoC-Window Distribution Shift: An Empirical Evaluation of LSTM-Based Models

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Data-driven State-of-Charge (SoC) estimation methods based on deep neural networks have shown strong performance under laboratory conditions. However, most existing studies train and evaluate models within a fixed SoC operating window, implicitly assuming that the training and deployment data share the same SoC range. In real-world applications, such as battery operation in the transport and energy sectors, the usable SoC window frequently varies due to usage patterns, charging strategies, and degradation, leading to systematic distribution shifts that are rarely evaluated.

This work investigates the impact of SoC-window distribution shift on deep learning–based SoC estimation. We introduce a window-shift evaluation protocol in which models are trained on data from two SoC windows and tested on a third, unseen window. Using long short-term memory (LSTM) networks as representative sequence models, we show that such models experience notable performance degradation under window shift compared to conventional fixed-window testing. These results indicate that increased model capacity can exacerbate overfitting to window-specific temporal patterns rather than improve robustness.

The results demonstrate that SoC-window distribution shift is a critical and previously underexamined source of error in deep learning SoC estimation. This study highlights the limitations of current evaluation practices and shows that strong fixed-window performance does not imply robustness under realistic operating conditions. The proposed evaluation framework provides a foundation for future research on window-agnostic and deployment-robust SoC estimation methods.

Operando Gas Analysis to Detect Lithium Plating in Li-ion Batteries during Fast Charging

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Lithium plating on graphite anodes during fast charging and at low temperatures is a major cause of capacity loss and a serious safety hazard in Li-ion batteries. Reliable detection and mechanistic understanding of plating are, therefore, essential for developing safe fast-charging protocols. The voltage plateau relaxation (VPR) method can detect plated lithium through a characteristic differential open-circuit voltage (dOCV) signature that arises as surface lithium chemically intercalates into graphite. While effective for detection, VPR alone provides no chemical insight into the interfacial reactions that accompany plating and stripping. Online Electrochemical Mass Spectrometry (OEMS) enables real-time quantification of gases evolving from electrode–electrolyte side reactions, offering a complementary chemical fingerprint of processes at the anode surface. To our knowledge, no prior study has combined OEMS with VPR to correlate gas evolution with the electrochemical signatures of lithium plating. In this work, we apply this dual approach to LFP/Graphite coin cells subjected to fast charging over a few cycles. During charge, enhanced gas evolution is expected under plating conditions due to electrolyte reduction on freshly deposited lithium metal. During relaxation, gas evolution profiles are correlated with the dOCV plateau to distinguish reversible lithium stripping from irreversible plating. We aim to identify distinct gas signatures for each regime, providing direct chemical evidence that complements electrochemical detection. These results are intended to support the development of improved diagnostic tools and safer fast-charging strategies for Li-ion batteries.

Correlating Electrochemical Responses and Structural Characteristics of Pulse-Induced SEI Evolution on Graphite Anodes

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The solid electrolyte interphase (SEI) on anodes plays a critical role in lithium-ion battery performance, yet its response to time-structured operating conditions remains insufficiently understood. Pulse charging is particularly relevant because the alternation between current-on and rest periods can modulate the build-up and relaxation of concentration gradients and polarization, as well as the progression of interfacial reactions at the anode/electrolyte interface. However, how pulse frequency and duty cycle affect SEI-related interfacial processes, and whether the resulting differences can be resolved through electrochemical responses, remains unclear.

In this work, graphite half-cells are used as a model system to investigate pulse-induced changes at the graphite/electrolyte interface. A controlled set of pulse protocols with different frequencies and duty cycles are applied to perturb interfacial processes. Electrochemical impedance spectroscopy (EIS) is used to monitor the evolution of interfacial impedance, while nonlinear frequency response analysis (NFRA) probes higher-order responses associated with nonlinear interfacial kinetics. Selected post-test samples are characterized to assess pulse-dependent structural characteristics of the SEI.

Electrochemical and structural readouts are integrated to trace how pulse temporal structure is encoded in SEI evolution on graphite anodes.

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Influence of initial ALD pulse sequence on surface reactions and electrochemical performance of NMC811

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Global deployment of lithium-ion batteries continues to increase, driven primarily by electric vehicles. Among cathode materials for electric vehicles, Ni-rich layered oxides such as LiNi0.8Mn0.1Co0.1O2 (NMC811) are widely used because of their high energy and power density. However, NMC811 suffers from capacity fade due to irreversible structural changes at high operating voltages. One promising strategy to mitigate these degradation mechanisms is the deposition of inorganic surface coatings by atomic layer deposition (ALD). While ALD enables precise control over coating thickness and uniformity, the surface reactions occurring during the initial ALD half-cycles on cathode powders remain poorly understood.

In this work, synchrotron-based in situ and operando ambient pressure X-ray photoelectron spectroscopy was employed to investigate surface reactions during AlOx ALD at 120 °C on NMC811 powder. The influence of precursor pulse sequence during the initial ALD cycle was studied by acquiring high-resolution spectra during pulsing of trimethylaluminum (TMA) and H_2O. The results show that the precursor sequence affects the early-stage surface evolution, while valence band analysis indicates differences in the uniformity of the resulting oxide layer. Electrochemical measurements were performed for coatings initiated either by a TMA or H_2O pulse. In full-cell configuration, both coated materials showed higher initial specific discharge capacity and improved long-term cycling stability than pristine NMC811. After 500 charge-discharge cycles, the capacity retention reached 82% for H_2O-NMC, 78% for TMA-NMC, and 71% for pristine NMC811.

Overall, this work improves the understanding of ALD surface chemistry on NMC811 powder and links the initial coating chemistry to electrochemical performance.

Operando synchrotron X-ray diffraction and imaging of solid-state lithium batteries

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Solid-state batteries are promising new battery technologies, which will offer a safer alternative to conventional lithium-ion batteries: the flammable organic solvent and fluoride-based salt will be replaced by a non-flammable solid electrolyte. In traditional LIBs, the liquid electrolyte conformally coats a porous electrode, maximizing the electrode/electrolyte contact area and creating an ionic transport path. In solid-state batteries instead, charge transport is a key challenge: electrodes should be dense to maximize the contact between particles, and the morphology should include percolating electronic and ionic pathways. While a continuous stack pressure is useful to address the first challenge, the latter is far mor complex.

We have built a custom-made setup compatible with beamline stages which hosts a 3 or 5 mm diameter in-situ battery cell, and monitors the pressure applied with an adjustable screw, while the potentiostat cables are connected. From spatially and time-resolved operando X-ray diffraction experiments we follow the structural changes in the active materials (using Rietveld refinement) as a function of time and position in the cathode layer. We combine this with X-ray computed tomography, to visualize morphology changes during charge-discharge, and at different applied pressures. We have utilized this setup in operando experiments on LiNiO2/Li3YCl6/Li-In cells at the DanMAX beamline (MaxIV) and at P21.1 (Petra III), revealing lithiation gradients and morphological variations under pressure. These findings can explain poor cathode utilization and capacity fading in new solid-state batteries under realistic conditions, informing the development of better cathode composites and more stable interfaces.

Probing electrolyte-dependent sodium storage in hard carbon electrodes

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Despite hard carbon being the preferred negative electrode in sodium-ion batteries, the sodiation process in the material remains debated due to its disordered structure. While many studies attribute variations in sodium storage to structural differences arising from synthesis, the role of electrolyte chemistry and charge rate is rarely considered in the same context. Here, we show that electrolyte choice and cycling conditions can influence the sodiation behavior and cycling performance of hard carbon.

By comparing carbonate- and ether-based electrolytes (Figure 1), clear differences in electrochemical performance are observed, suggesting distinct storage pathways. To elucidate these differences, small- and wide-angle X-ray scattering measurements performed at different degree of sodiation reveal changes in structural evolution during cycling. Variations in the scattering signal correlate with changes in electron density contrast between micropores and surrounding carbon matrix, enabling tracking of pore filling during sodiation. The results indicate that electrolyte and charge rate influence the sodiation process, with earlier intercalation in ether-based electrolytes, and reduced pore utilization at a higher charge rate.

To further investigate these effects, operando synchrotron X-ray total scattering measurements have been performed to probe local atomic structure during cycling. The results will provide insights into changes in Na–C correlations, graphene layer spacing, and possible co-intercalation. These are complemented by X-ray photoelectron spectroscopy to examine electrolyte-dependent surface chemistry and interphase formation.

Together, these approaches link chemical and structural information across length scales, providing new insight into electrolyte-dependent sodium storage mechanisms in hard carbon.

Methods for investigating state of health of used EV battery modules

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Background

Information about a battery's state of health (SoH) is essential to enable safe operation of both smaller and larger batteries. Additionally, it is vital to accurately diagnose SoH for batteries intended for repurposing or second-life use. Establishing SoH currently requires time-consuming and costly battery diagnostics routines to ensure that the used batteries are suitable for their new application. In this work, we have explored two different diagnostic techniques on battery modules, which are most commonly used on single cells; galvanostatic intermittent titration technique (GITT) and intermittent current interruption (ICI).

Results

We performed GITT and ICI measurements on battery modules from two different electric vehicles (EVs). Six of the battery modules were from a relatively new EV with estimated SoH at 96%, while the other six modules were estimated to have 84% SoH. This provided us with battery modules with very different user history and degradation. Figure 1 shows data from two different modules. Additionally, impedance measurements were conducted on cells within the modules to compare with the resistances obtained from GITT and ICI.

Figure 1: ICI and GITT of two different modules, one at 84% SoH and the other at 96% SoH.

Conclusions

The obtained data indicate that ICI might have certain advantages over GITT for diagnosing a battery's SoH. However, it is clear that accurate information is challenging to obtain on module level with both methods, and complementary techniques such as electrochemical impedance spectroscopy (EIS) are required for more detailed diagnostics.

Correlation between electrode's structural and mechanical behaviour using operando XRD and dilatomtery

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Understanding the relationship between crystal structure evolution of electrode active materials and the resulting mechanical behavior at the electrode level is essential for stabilizing battery performance under realistic operating conditions. In this work, operando X-ray diffraction (XRD) is combined with operando electrochemical dilatometry to directly correlate phase transitions with electrode volume changes during cycling. The versatility of this approach is demonstrated across both lithium- and sodium-ion battery systems.

For Mg-doped Ni-rich layered oxide (NMC811), operando XRD revealed a two-phase transition pathway (H1–H2–H3). Complementary dilatometry measurements showed faster stabilization of electrode volume changes, indicating that Mg incorporation suppresses structural strain and promotes faster stabilization during cycling, ultimately improving long-term electrochemical performance. These results demonstrated how targeted cation substitution can effectively mitigate degradation associated with repeated lattice breathing.

For biomass-derived hard carbon anodes, the combined operando approach revealed distinct sodiation mechanisms regulated by pore network structure. Variations in precursor-dependent microstructure strongly influence irreversible capacity loss, electrode expansion, and cycling stability. In particular, higher defect density and surface area lead to increased initial capacity loss, while enhanced mesoporosity improves structural stability over prolonged cycling.

Overall, this study demonstrates that coupling operando structural and mechanical characterization provides key insights into degradation mechanisms and explains performance differences between modified and pristine materials, enabling the rational design of more durable and scalable battery electrodes.

Sodiation mechanism in biomass-derived hard carbons studied by operando Raman spectroscopy

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Hard carbons derived from sustainable biomass are among the most promising anode materials for sodium-ion batteries, but their sodium storage mechanisms is not fully understood due to structural heterogeneity. Post-mortem characterisation is insufficient to resolve these mechanisms, making operando techniques essential. In this work, operando Raman spectroscopy in an EL-Cell [1] configuration is used to investigate structural changes during electrochemical sodiation and desodiation in different biomass-derived hard carbons: peat-derived carbons [2] and the commercial Kuranode [3].

These materials demonstrate excellent reversible capacities of 350 [2] and 371 mAh g^{-1} [3], respectively. Operando Raman heatmaps for the materials show systematic and reversible spectral changes upon cycling (Figure a,b). With increasing sodiation, the D- and G-bands shift closer together and both bands' full width at half maximum become broader, indicating growing lattice strain and local structural disorder. The D/G intensity ratio stays largely constant throughout sodiation and desodiation in both materials.

The stability of the D/G ratio indicates that sodium insertion does not generate or reduce graphitic defects. Combined with the full reversibility of all spectral changes, this suggests sodium adsorption at defect sites and pore filling mechanism. The consistent behavior observed for the structurally distinct hard carbons suggests these Raman spectra may be a general indicator of sodium storage in disordered carbons.

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From Screening to Mechanism-Informed Analysis: A Standardized High-Throughput Electrochemistry Platform for Redox Species Discovery

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With growing concerns over energy shortages and environmental issues, renewable energy sources such as hydropower, wind power, and solar power are receiving increasing attention. Flow batteries (FBs) have decoupled power and energy, high safety, long lifetime and good scalability, holding greater potential for long-duration large-scale energy storage applications. Redox-active species, which are molecule or ions that can reversibly covert between oxidized and reduced states, play an important role in FBs. Systematic evaluation of redox-active species is crucial for developing next-generation energy storage materials, yet traditional electrochemical studies remain constrained by throughput limitations. We proposed a high-throughput platform HT-EChem integrating cyclic voltammetry (CV) into a 96-well plate format, enabling rapid, reproducible measurements of multiple samples and systematic acquisition of large-scale, low-noise electrochemical data. As a demonstration, we focused on iron complexes and organic redox active materials, revealing their fine-tuned shifts in redox potentials with pH variations and stability trends, thereby elucidating their mechanistic pathways. Notably, Fe–PDTA shows dual reduction peaks due to an electrochemical–chemical process with structural rearrangement, whereas Fe–EDTA and Fe–DTPA display single peaks. The systems allow fast measurements of the Pourbaix diagrams of molecular species. When coupled with high-throughput synthesis, the platform allows generation of datasets to provides a robust foundation for machine learning models and density functional theory calculations, enabling data-driven active molecular design and predictive understanding.

Revealing electrolyte-dependent behaviour of Sn-based conversion-alloying anodes for Na-ion batteries

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SEI stability in NIBs is more challenging due to the higher solubility of Na-containing interphase species in carbonate-based electrolytes. The electrochemical performance of Sn-based conversion alloying (CA) anodes was found to be significantly worse in carbonate-based electrolytes compared to glyme-based electrolytes. Moreover, the reaction mechanisms of Sn-based CA anodes are not yet fully understood. In particular, the extent to which conversion and alloying reactions proceed sequentially or concurrently, as well as the reversibility of the conversion step.
In this research, the working mechanism of the anodes (SnO, SnS, SnSe) was studied. Differences in conversion and alloying reaction mechanisms and their progression caused by carbonate and glyme-based electrolytes were established. Influence of electrolytes on electrochemical performance, interfacial processes at the electrode, and particle morphology were analysed.
The reversibility of the conversion reaction was found to be different in different anodes (SnO, SnS, SnSe). The fundamental mechanism of (de)sodiation of oxide (SnO) was different from chalcogenides (SnS, SnSe). The effect of the electrolyte on the mechanism of the reversibility was visible, but the progression was not significantly different. The alloying component of the (de)sodiation in all anodes differed drastically between the two electrolytes, with carbonate showing much worse (de)alloying. The postmortem analysis of all the anodes with carbonate showed a much higher content of NaF as well as a low content of free Sn. Rapid capacity fade of anodes in carbonate-based electrolyte was primarily due to inaccessibility of (de)alloying past first discharge and unstable SEI formation.

Probing Multi-Electron Redox in Organic Cathodes via X-ray Absorption Spectroscopy and Resonant Inelastic X-ray Scattering

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Conventional transition-metal-oxide cathodes (e.g., NMC, NCA, LCO, LFP) are constrained by cost, resource concentration, and environmental impact. In contrast, organic cathodes composed of earth-abundant elements (C, H, O, N, S) offer sustainable synthesis, lower cost, and molecular tunability. Their programmable frameworks enable rational control of redox potential and capacity through functional group engineering, providing a compelling alternative to rigid inorganic lattices.[1-3] Despite promising reports demonstrating high capacity, rate capability, and cycling stability, the fundamental redox mechanisms in organic cathodes remain insufficiently resolved. Prior studies largely attribute charge storage to localized bond rearrangements without phase transitions, yet lack atomistic insight from advanced spectroscopy. Here, we address this gap by employing X-ray Absorption Spectroscopy (XAS) and Resonant Inelastic X-ray Scattering (RIXS) at the O, N, and C K-edges to investigate a benchmark organic cathode delivering higher capacity ~325–337 mAh g^{-1}(ref. Fig).[4-5]

State-of-charge-dependent XAS reveals the evolution of unoccupied electronic states, identifies redox-active moieties, and tracks ion coordination environments. Complementary RIXS measurements uncover bonding reorganization, intermediate species formation, and subtle electronic–structural dynamics. These combined analyses elucidate the sequence of electron transfer, confirm the formation of radical intermediates, and clarify the roles of C=O and C=N groups in a multi-electron redox process. Notably, vibronic energy-loss features in RIXS provide direct evidence of polaronic states and transient radical species. This pioneering work establishes a comprehensive, atom-specific picture of energy storage in organic cathodes and demonstrates how advanced spectroscopy can uncover mechanistic pathways, marking a significant step toward rational design of next-generation sustainable battery materials.

Linking Material Properties to Fast-Charge Performance in Battery Anodes

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Fast charging of lithium-ion batteries is often limited by coupled transport processes arising in commercially relevant thick electrodes, making it difficult to isolate and quantify intrinsic material-level limitations of anode materials. This work establishes an experimental framework to quantify the fast-charge capability of anode materials while minimizing electrode- and cell-level transport effects. Ultra-low loading electrodes are used to suppress ion transport limitations and micro-reference electrode to minimize overpotential in the electrolyte and remove overpotential contribution from counter electrode. The methodology enables determination of the maximum charging rate achievable before the onset of detrimental side reactions such as lithium plating.
Electrochemical characterization techniques are applied to distinguish whether rate limitations originate from charge-transfer processes at the particle surface or lithium transport within the active material bulk. Based on these insights, material design strategies targeting enhanced fast-charge performance are explored, including modifications of primary particle size such as for example, degree of graphitization, surface area of the material, coating thickness and degree of coating.
In this work, we will present first results on how different material bulk and surface properties influence charge transfer kinetics and solid-state lithium diffusion, and how these processes govern the fast-charging performance of anode materials.

Operando Gas Evolution Dynamics in High-Temperature Aged Commercial Tesla 21700 Lithium-ion Cells

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Lithium-ion batteries (LIBs) are rapidly expanding across the electric vehicle market and are on the verge of widespread adoption in large-scale grid storage.[1,2] Each of these applications requires a fine balance among key performance factors, including energy density, power output, lifespan, cost, safety, and environmental impact. However, operating LIBs near their physical limits makes safety a persistent critical concern, underscored by frequent reports of thermal runaway, smoking, and fires. Identifying and mitigating internal side reactions is therefore vital to improving battery performance and reliability. A primary degradation pathway during battery aging is electrolyte decomposition, which generates flammable, explosive, and toxic gases while increasing internal cell pressure.[3] Consequently, quantifying gas evolution in commercial cells is essential for ensuring safe operation. Electrochemical mass spectrometry has emerged as a powerful diagnostic tool for this purpose, offering the high sensitivity and specificity needed to detect and quantify minute gas species originating from interfacial side reactions at the electrode surface.[4] In this work, we present an online electrochemical mass spectrometry (OEMS) investigation of gas evolution in commercial 21700 Tesla cells. We compared cells aged to 70% state-of-health (SOH) via pulse charging at 45°C against cells at 90% SOH, establishing direct links between gas generation with C-rates and internal impedance growth.

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The role of lattice and surface oxygen in charge compensation of a P2 sodium-ion cathode

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P2 layered transition metal oxides are promising cathode materials for sodium-ion batteries due to their high operating voltages, moderate to high specific capacities, and reliance on earth-abundant elements. However, their practical application is hindered by intrinsic structural instabilities, including Mn^{3+}-driven Jahn–Teller distortions and irreversible P2–O3 phase transitions during deep cycling [1]. These processes are closely linked to charge compensation mechanisms across the surface and bulk, yet their atomistic origins remain insufficiently understood.

Here, we investigate the P2-type cathode $Na_{0.67}Mn_{0.5}Fe_{0.45}Mg_{0.05}O_2$ (NMF-Mg), cycled to well-defined states of charge (SOCs) between 4.2 V (charge) and 1.5 V (discharge) over two cycles. A combination of surface- and bulk-sensitive spectroscopies probes charge compensation across multiple length scales. Depth-resolved photoelectron spectroscopy reveals a systematic O 1s binding energy shift with SOC, indicating strong coupling between electrochemical state and the oxygen coordination environment from the topmost surface to the near-surface bulk.
Complementary Fe and Mn K-edge X-ray absorption spectroscopy shows only subtle edge shifts and constant pre-edge positions, while increased pre-edge intensity at high charge and deep discharge suggests enhanced local disorder of MO_6 octahedra rather than evident changes in formal oxidation states. Oxygen K-edge RIXS further reveals the emergence of molecular O_2-like species at 4.2 V, which are depleted upon discharge to 1.5 V.

Together, these observations suggest that oxygen redox activity and complex charge redistribution involving oxygen ligands play a significant role in charge compensation, which may obscure conventional transition metal redox fingerprints.

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Novel In-Plane Permeability Measurement Rig for Commercial Battery Electrodes

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Electrolyte motion induced salt gradient (EMSI) has recently been study for cylindrical 18650 cells and any other larger formats, such as 4695 cells. EMSI is a degradation mechanism that originates from coupled in-plane electrolyte motion and through plane electrolyte salt concentration gradient during charging and discharging of battery electrodes. This motion causes electrolyte salt depletion towards the up and lower edges of the jelly roll (positive and negative terminals, respectively) and enrichment in the centre, leading to cell capacity fade, increased ionic resistance and overtime localized lithium plating. The mechanistic origin of the electrolyte salt gradient was assumed to be from the electrolyte flow, preferentially in the anode than the cathode electrode, due to graphite particle's structure and orientation, that results in higher in-plane electrolyte permeability than in less porous spherical cathode particles. We, therefore, developed a novel gas flow based in-plane permeability measurement tool, to measure the porous media's permeability. Among the measured commercial cells so far, the in-plane permeability of beginning of life Samsung 35E is more than 4 times higher than that of the cathode electrode. However, this ratio is different for commercial LG-MJ1 cells, showing that the in-plane permeability is different for different electrode and cell designs. Finally, electrodes from other commercial cells and cell chemistries will be presented and discussed, to match the anode and cathodes by in-plane permeability measure.

Transmission electron microscopy of beam sensitive battery electrodes

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Aberration corrected transmission electron microscopy (TEM) can provide information with atomic resolution about structure, morphology and chemical composition using imaging, spectroscopy and diffraction. TEM is therefore a key methodology to understand the complex relationships between materials and properties in batteries. A fundamental challenge is that many of the electrode components, and in particular the solid electrolyte interfaces (SEIs), are electron beam sensitive. Heating and radiolysis often destroy the inherent structure and chemistry of SEIs and other electrode components.

Figure 1(a) shows a SiNx particle inside an electrode cycled 200 times. The active particle is surrounded by a thick SEI, and in Fig. 1(b) the region is mapped by electron energy loss spectroscopy (EELS). After mapping (Fig. 1(c)) most of the SEI is destroyed due to beam damage. Any quantifications of the SEI are therefore difficult, as the inherent structure and chemistry of the SEI sub-layers are likely modified and destroyed before the information can be collected.

In the present work we will demonstrate how electron beam damage can be reduced or totally avoided by the new possibilities offered by direct electron detectors and advanced dose modulation systems. This progress is possible through advanced pulsing of the electron beam through a dose modulation system, combined with ultra-fast EELS mapping, multiple frames and fast direct detectors with high dynamic range.

Understanding hard carbon anodes with in situ and operando studies

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Hard carbon is the state of the art anode material for sodium ion batteries. It is produced from both fossil and biomass carbon sources and can offer comparable capacity, cyclability and rate performance to graphite in lithium ion batteries. Unfortunately, the properties of the hard carbon are highly influenced by the feedstock and processing route, as well as the electrolyte used in the cell. We have set out to understand the relationships between feedstock, processing route, electrolyte and electrochemical properties at the chemical structure level using in situ and operando XRD and total scattering methods to study synthesis and cycling of hard carbons from different sources and with different electrolytes.

Lithium-Ion Chemical Potential as a Thermodynamic Descriptor for Solid Polymer Electrolytes

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Lithium-ion chemical potential (μLi+) has recently emerged as an important thermodynamic descriptor governing Coulombic efficiency and interfacial stability in liquid electrolytes. However, its role in solid polymer electrolytes (SPEs) remains largely unexplored, despite the fundamentally different chemical environment and ion–polymer interactions present in these systems.

Here, we investigate lithium-ion thermodynamic stabilization across a range of SPE chemistries, with a particular focus on poly(ethylene oxide) (PEO) spanning molecular weights from several hundred to over one million g/mol, as well as alternative polymer backbones including poly(trimethylene carbonate) (PTMC) and poly(caprolactone) (PCL). LiTFSI is used as the primary lithium salt at fixed polymer–salt weight ratios to enable direct comparison across different polymer systems.

Preliminary results reveal a strong molecular-weight-dependent trend in lithium-ion thermodynamic stabilization in PEO-based electrolytes. Below approximately Mn ≈ 1000 g/mol, increasing polymer molecular weight leads to increasingly favorable lithium-ion stabilization, while above this regime the trend gradually approaches a plateau-like behavior. These trends are consistent with previous spectroscopic studies. Comparisons across different polymer chemistries further reveal that PTMC exhibits the highest lithium-ion chemical potential, PCL shows intermediate behavior, and PEO exhibits the lowest chemical potential, indicating distinct lithium-ion stabilization environments across different polymer chemistries, in agreement with reported coordination trends.

Previous studies have shown that ion coordination environments strongly influence ion transport in polymer electrolytes. In this context, lithium-ion chemical potential emerges as a complementary thermodynamic descriptor for understanding ion transport, plating/stripping behavior, and electrochemical performance in SPEs, particularly in anodeless solid-state batteries.

Looking at Graphite from a Different Angle: Insights into the Mechanism of Co-intercalation Processes

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Graphite is the commercial choice of anode material for Li-ion batteries due to its low cost, abundance, and well-established processing. Its electrochemical behavior has been traditionally explained using the Rüdorff and Daumas–Herold models, which interpret ion storage as a staged intercalation process. However, these models do not fully explain the detailed mechanism of co-intercalation. The use of operando techniques, such as operando X-ray diffraction, allow us to directly observe the structural changes in graphite during electrochemical cycling and, therefore, can help to determine the operating mechanism of active materials.

In this study, we directly compare the diffraction pattern during operation and electrochemical behavior of different electrolytes in sodium- and potassium-ion batteries using graphite as the anode. While previous operando diffraction studies have mainly focused on the evolution of the 002 peak to confirm intercalation, the present work expands the analysis to the 001 and 101 peaks. By doing so, we aim to provide a comprehensive understanding of how the solvated ions move through the graphite layers.

The diffraction pattern, particularly at low angles, indicates the co-intercalation of molecules much larger than previously thought, which may interfere with the symmetric movement of the graphite layers observed during Li-ion intercalation in conventional systems. These findings enhance our understanding of how post-lithium batteries store energy, which supports the movement towards the use of more sustainable energy systems.

Highly reliable and highly processable hybrid solid electrolyte for K-ion Batterie

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Solid polymer electrolytes are now widely studied to develop safer and greener energy storage systems and are very interesting for metal-ion batteries due to their very low cost, great sustainability and compatibility with continuous processing methods. However, they are suffering from very low ionic conductivity at low temperatures (under 50°C). On the other hand, Inorganic solid electrolytes have high ionic conductivity at room temperature but suffer from terrible processability, extremely bad contact between electrodes and electrolyte and most of the time from small electrochemical stability window.
In this work, we have developed a mix of a sand based inorganic part such as KMS (K2+xMg1-x/2SiO4) and an ether polymer like polyethylene oxide to synergistically profit from the advantages of both types of electrolytes forming a layer easy to process, with great ionic conductivity at room temperature, great stability window, highly reliable and cheap. We have studied various formulation of membrane with different amounts of KMS, different polymer types, temperature and process to determine the electrochemical performances of this composite membrane and then we have shown the capabilities of this electrolyte to cycle in a Half-cell configuration using KMO (Manganese based oxide cathode material) or electroactive organic cathode materials versus potassium metal electrode.

Interphase Formation and Degradation Pathways in Lithium-metal Solid-State Batteries

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Lithium metal solid-state batteries offer compelling energy density and safety advantages over conventional lithium-ion batteries, but degradation at the solid-solid interfaces remains a critical challenge limiting their performance and lifetime. In particular, the interface between the lithium metal anode and the sulphide solid-state electrolyte Li_6PS_5Cl (LPSC) is unstable and degradation at this interface will occur through complex coupled mechanical, chemical, and electrochemical pathways. In this work, we investigate interphase formation and growth at the Li/LPSC interface using electrochemical characterization combined with multimodal X-ray imaging to directly correlate the electrochemical signatures with structural and chemical changes. Overall, the results show that chemically and electrochemically driven degradation produce distinct chemical and morphological signatures of the interphase, more heterogeneous and structurally complex than commonly assumed.

Emergent Transition-Metal Ordering in Mn-Rich P2 Sodium-Ion Cathodes: Pathway to Reversible Oxygen Redox

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Large-scale energy storage is essential for enabling renewable energy integration and grid stability. Sodium-ion batteries (SIBs) are promising for stationary applications due to the abundance and low cost of sodium and transition metals. Among cathode materials, Mn-based P2 layered oxides are particularly attractive; however, their performance often degrades under high-voltage operation required for increased energy density.

Here, we report a Mn-rich P2-$NaMnNiCoO_2$ cathode (low Ni/Co content) exhibiting stable high-voltage electrochemical performance without the use of aliovalent dopants or surface coatings. A scalable, surfactant-free synthesis route yields homogeneous precursors that promote intrinsic structural ordering in the final material. Phase evolution during synthesis is tracked by in-situ high-temperature X-ray diffraction (HT-XRD), confirming controlled formation of the P2 structure. Ex-situ synchrotron XRD (ESRF) reveals phase purity and superlattice reflections associated with Na^+/vacancy and transition-metal ordering, supported by SAED and HR-TEM analysis.

Operando synchrotron XRD demonstrates a fully reversible solid-solution reaction during the initial cycle up to 4.4 V vs Na^+/Na, with no detectable phase transitions or stacking disorders. The cathode delivers an initial discharge capacity of 113 mAh g^{-1} and 92% capacity retention after 50 cycles, maintaining stable cycling and minimal voltage hysteresis over extended operation. Strong rate capability is observed across a wide range of current densities.

These results highlight intrinsic ordering as a key strategy to stabilize high-voltage redox in Mn-rich P2 cathodes, offering a scalable pathway toward sustainable SIBs.

Oxygen-Ion Batteries: A next-generation solid-state energy storage solution

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Oxygen-Ion Batteries (OIB) are a next-generation all-solid-state battery technology invented at TU Wien, Austria. This new type of battery exploits the oxygen non-stoichiometry of mixed ionic-electronic conducting materials such as $La_{0.6}Sr_{0.4}FeO_3$-δ, $Ca_{0.3}Sr_{0.7}Fe_{0.92}Ti_{0.08}O_3$-δ and $La_{0.5}Sr_{0.5}Cr_{0.2}Mn_{0.8}O_3$-δ for multi-hour energy storage. Its ceramic nature makes the battery non-toxic, non-flammable, non-explosive and thus inherently safe. In addition to the two storage electrodes, the OIB exhibits a third so-called “recovery” electrode, via which reversible capacity losses can be regenerated. Thereby the battery’s lifespan is significantly extended. Moreover, this third electrode enables monitoring the state of each working electrode separately even during charging and discharging, providing the basis for optimized battery performance.

The Christian Doppler Laboratory for Oxygen-Ion Batteries at TU Wien conducts research on powder-based OIBs as an industrially scalable variant of this technology (see Figure). This contribution provides an overview of this emerging battery technology, emphasizing cell design, cell performance, as well as industrially scalable production methods like tape-casting, screen printing and inkjet-printing of ceramic materials.

So far multiple prototypes have been developed, including a multi-cellular system of 5×5cm² powder-based cells manufactured via tape-casting and screen-printing. Electrochemical characterization through charge-discharge cycling at operating temperatures of 450–550°C demonstrated coulombic efficiencies exceeding 99% and round-trip efficiencies up to 82%.

By further improving electrode materials and scalable production techniques, OIBs will become a safe, versatile, and sustainable alternative to existing technologies in large-scale energy storage.

A new borate-based fluorine-free electrolyte for Na-ion batteries

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State-of-the-art Na-ion battery electrolytes are mostly inherited from the Li-ion technologies and contain highly fluorinated chemicals that are toxic, corrosive and difficult to recycle. For Na-ion batteries to offer a sustainable alternative for Li-ion batteries, more sustainable, fluorine-free electrolyte systems should be investigated. While some fluorine-free systems have already been reported, they suffer from poor initial Coulombic efficiencies which affect the performance of the battery cells.

In this work, a new borate-based fluorine-free electrolyte was developed and its physicochemical and electrochemical properties were investigated. The salt was synthesised and its composition and purity were confirmed using nuclear magnetic resonance, Fourier transform infrared spectroscopy (FTIR) and thermogravimetric analysis. The salt showed good solubility in the selected solvent with the moderate ionic conductivity of ~2 mS/cm. The electrochemical performance of the electrolyte was tested through galvanostatic cycling and cyclic voltammetry. The results show that the electrolyte suffers from non-passivating salt decomposition at 2.4 V that leads to poor cycling performance. The decomposition can be prevented by adding 2 wt% of electrolyte additive which reduces before the salt decomposes during the first cycle. X-ray photoelectron spectroscopy, electrochemical impedance spectroscopy and FTIR results show that the additive changes the formation, composition and thickness of the solid electrolyte interphase (SEI) considerably and hinders the electrolyte decomposition at higher voltages, leading to improved performance.

As a conclusion, the work presents a new fluorine-free electrolyte for Na-ion batteries, and shows that great improvements can be gained in the electrolyte performance with well-selected additives.

P2-type Na0.67(Ni0.33Mn0.67)O2 Na-ion cathode: Effect of low and high temperature synthesis on the electrochemical performance

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P2-type Na0.67Mn0.67Ni0.33O2 (NMNO) is a potential cathode for Na-ion batteries. In this study, we synthetized and characterized NMNO by a low temperature synthesis (coprecipitation of hydroxide precursor followed by sodiation) and compared this with high-temperature synthesis of NMNO. We used earlier developed method low-temperature synthesis method for Mn-rich cathodes1-2. Characterization was done using e.g., X-ray absorption spectroscopy (XAS), ICP-OES, SEM-EDS, and in situ XRD. Galvanostatic cycling was carried out in the voltage range of 2.1-4.5 V versus Na+/Na at the current rate of C/5 rate (1 CNMNO = 173 mAh g -1).

Morphology of NMNO was spherical. Overall, our results demonstrate that a low temperature synthesis route significantly enhances the electrochemical performance of NMNO during initial cycling (up to 80 cycles). However, upon extended cycling (beyond 100 cycles), cathode active materials synthesized via both low and high temperature routes exhibit Mn reduction at the particle surface, as revealed by surface sensitive soft XAS in total electron yield (TEY) mode. This surface Mn reduction triggers pronounced surface degradation, ultimately leading to progressive capacity fading.

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Factors influencing ion transport in sodium halide solid ionic conductors

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Sodium ion solid ionic conductors based on chloride chemistries are currently being investigated as promising candidates for electrolytes or catholytes in solid-state batteries. In particular, significant efforts have been devoted to the design of sodium containing ternary chlorides with nominal composition Na_xMCl_6 (M = In^{3+}, Er^{3+}, Zr^{4+}, Nb^{5+}, Ta^{5+} or Sb^{5+}) [1-4], and mixed-anion compounds with nominal compositions related to $NaMXCl_4$ (M = Nb^{5+} or Ta^{5+}).[5-7]

Despite the considerable improvements in ionic conductivity reported for these materials, the factors governing sodium transport remain incompletely understood. In this presentation, we focus on the chemical, structural and microstructural features that could be behind ionic mobility in these chloride-based systems. Particular attention is given to the role of the defect chemistry, crystallinity and electronic configuration of the metal cation. By correlating experimental observations with structural descriptors, we suggest some parameters that play a role in ionic conductivity and hope to provide insights to guide the rational design of next-generation sodium solid electrolytes.

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Exploring novel halide and oxyhalide solid electrolytes: from doping strategies to amorphous systems

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Halide -based solid-state electrolytes (HSSEs) have emerged as a favorable candidate for next-generation solid-state batteries (SSBs) due to their excellent electrochemical stability window, high ionic conductivity, and compatibility with high voltage cathodes. Compared to sulfide-based SSEs, HSSEs offer improved chemical stability, scalability, and moisture tolerance, making them attractive for large-scale applications. However, their commercialization is constrained by inherent mechanical limitations and interfacial issues with cathodes as well as Li metal anode. Additionally, the potential for synthesizing new materials to achieve high ionic conductivity, electrochemical stability, and scalability for future energy storage devices has not been fully explored.

Amorphous solid electrolytes with dual anion hold great promise for achieving favorable performance, such as high ionic conductivity and good compatibility with electrodes within solid state batteries. Their amorphous nature reduces grain boundary resistance, facilitates isotropic ionic transport, and enhances mechanical properties, while maintaining good electrode compatibility. This study investigated new novel amorphous nitride oxyhalide electrolytes ($Li_{3+x}NbN_xO_yCl_{5-x}$ and $Li_{3+x}TaN_xO_yCl_{5-x}$) synthesized via mechanochemical methods. Preliminary studies indicate the amorphous structure of the materials and demonstrate ionic conductivities in the range of ~10^{-3} S/cm. Different compositions and doping levels were investigated to optimize structural and electrochemical properties.

These findings suggest that amorphous nitride–oxyhalide electrolytes are promising candidates for solid-state battery applications, offering both improved ionic conductivity properties and improved mechanical robustness. Ongoing work focuses on further composition tuning and detailed electrochemical evaluation to confirm their potential as next-generation solid-state electrolytes.

Agarose gel electrolyte stabilizes zinc anodes suppressing hydrogen evolution monitored by operando electrochemical mass spectrometry.

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Aqueous zinc-ion batteries (ZIBs) are a promising technology for grid-scale energy storage. However, performance is limited by interfacial instability at the Zn anode. This interface is affected by parasitic reactions, dendrite growth, corrosion, and by-product formation. In particular, the hydrogen evolution reaction (HER) is a key parasitic process, causing electrolyte consumption, gas formation, and non-uniform zinc deposition, accelerating degradation and shortening cycle life [1].
In this work, an agarose-based GPE crosslinked with boric acid was developed to regulate the Zn-electrolyte interface. The GPE exhibits good mechanical properties and a wider electrochemical stability window than the 2 M $ZnSO_4$ liquid electrolyte, reaching 2.2 V compared to 1.75 V. The system delivers improved zinc plating-stripping efficiency in asymmetric cells at high current densities and areal capacities of 4 and 8 mA cm^{-2}- mAh cm^{-2} (~98-99%), together with stable symmetric cycling for over 4500 h in pouch cells. Operando differential electrochemical mass spectrometry (DEMS) directly reveals a significant suppression of HER in the presence of the GPE, particularly during the initial stages of deposition.
These results demonstrate that agarose-based gel polymer electrolytes effectively stabilize the Zn anode interface by suppressing HER and associated parasitic reactions, leading to improved efficiency and cycling stability. DEMS provides direct evidence of HER mitigation [2], offering key insight into the interfacial processes governing Zn anode parasitic reactions.

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Transport properties of amorphous Li7La3Zr2O12 thin-films as solid-state electrolytes

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Crystalline garnet LLZO (Li7La3Zr2O12) is considered a key contender for solid battery electrolytes due to high Li ion conductivity (10-3 S/cm) and a wide electrochemical stability window (6 V). However, challenges with processability and device integration hinder commercialization, due to high annealing temperature (up to 1100°C) with low reproducibility and large grain-boundary volume, thus prone to dendrite growth and early battery failure. Amorphous films are a promising alternative with high uniformity and density, low processing temperatures and nano-sized grains that may mitigate dendrite issues and increase the critical current density (CCD) of the battery.
In this work, we investigated amorphous LLZO (am-LLZO) thin films to establish correlations between structural characteristics and transport properties. Am-LLZO thin films were prepared with radio frequency magnetron sputtering (RF sputtering). The effects of processing parameters, including varying lithium concentration and deposition temperature, were investigated to understand their influence on film properties. Bonding structure and chemical composition were analysed using Fourier-transform infrared (FTIR), Raman spectroscopy and ionic transport evaluated using temperature-dependant electrochemical impedance spectroscopy (EIS).

Safer sodium-ion batteries by non-flammable, PFAS-free sulfone-based electrolytes

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As Europe continues its transition to renewable energy, the growing demand for energy storage raises significant concerns regarding the secure supply of critical raw materials (CRMs), such as lithium, copper, and cobalt. Sodium-ion batteries (SIBs) offer a CRM-free alternative, but their electrolyte formulations still rely on highly flammable solvents and toxic components that also pose severe hazards should there be e.g. a thermal runaway.

Here, we present a comprehensive investigation of a non-flammable PFAS-free electrolyte for SIBs utilizing ethyl methyl sulfone combined with the salt sodium bis(fluorosulfonyl)imide (NaFSI). In addition, we use non-toxic additives and diluents to facilitate formation of stable electrolyte/electrode interfaces/interphases and to lower the electrolyte viscosity.1

First, the ionic conductivity and viscosity were determined to assess dynamic properties. Second, the electrochemical behavior of Na||Hard carbon half-cells and Hard carbon||Prussian White full cells was observed via galvanostatic cycling at ambient temperature. Finally, flammability tests were conducted to demonstrate the superior safety vs. conventional electrolytes.

Overall, our findings indicate that sulfone-based electrolytes offer a promising and inherently safer pathway for the development and operation of next-generation SIBs.

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Acetonitrile as an additive for increased conductivity of aluminium battery electrolytes

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Aluminium carbon batteries are potentially low cost, durable and easy to recycle next generation batteries, based on an aluminium anode and a graphite cathode. Ionic liquids based on 1-Ethyl-3-methylimidazolium chloride ([EMIm]Cl) and aluminium chloride ($AlCl_3$) are typical electrolytes for aluminium batteries. In this work, the polar aprotic solvent acetonitrile (CH_3CN) is added to the ionic liquid as a potential conductivity enhancer. Acetonitrile is hypothesized to increase the conductivity by reducing the interaction between ionic species in the electrolyte, reducing the overall viscosity. The electrolyte conductivity for different concentrations of acetonitrile is measured by electrochemical impedance spectroscopy in symmetrical PAT-cells™, using molybdenum electrodes. Experimental results are compared to predictions of conductivity obtained by molecular dynamics simulations. Changes in the electrolyte composition after addition of acetonitrile is measured with Raman spectroscopy and ^{27}Al NMR.

Inorganic Coatings of Sulfide-based Solid-State Electrolytes through Atomic Layer Deposition (ALD)

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Solid-state batteries (SSBs) are regarded as a promising next-generation energy storage technology, offering a safer, more sustainable, and potentially cost-effective alternative compared to conventional Li-ion batteries (LIBs). The key component for high-performing SSBs is the solid-state electrolyte (SSE) with targeted properties (such as electrochemical stability window, performance, and safety). However, introduction of SSE also brings new challenges related to ionic conductivity, processability, recyclability, and the interface between the active material and the SSE needs to be carefully controlled. These challenges are addressed with the FUNCY-SSB (FUNctional Coatings of sulfide electrolYtes for lithium Solid-State Batteries) project. The presented work explores synthesis and characterization of lithium thiophosphates (LPS, such as Li7P3S11 and Li7PS6) as SSEs, and the synergistic effect of functional coating of LPS in combination with different inorganic materials (such as TiO2 and Al2O3) through atomic layer deposition (ALD). In addition, the work assesses the life cycle impacts of the coated LPS material production and identifies key environmental hotspots across the production routes.

Figure 1. a) The FUNCY-SSB approach. b) ALD process of TiO2 deposition on LPS powder. c) Electrochemical impedance spectra of pristine Li7P3S11 (LPS), TiO2-coated LPS, and LPS subjected to ALD conditions without pulsing the precursors.

From spent lithium iron phosphate to aqueous zinc-ion battery cathodes

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Rechargeable lithium-ion batteries (LIBs) dominate the portable electronics and electric vehicle markets due to their high energy density and long cycle life. Among LIB cathode materials, lithium iron phosphate ($LiFePO_4$, LFP) is widely utilised due to its low cost, stability, long cycle life, and improved safety. However, the growing production of LFP-based batteries is expected to generate substantial quantities of spent electrode materials. Conventional recycling routes for LIB cathodes are often energy-intensive and environmentally demanding, motivating the development of alternative reuse strategies for battery waste valorisation. Furthermore, the robust olivine crystal structure of LFP remains stable after delithiation, making $FePO_4$ (FP) a promising ion-host material for alternative battery chemistries.

Rechargeable aqueous zinc-ion batteries (AZIBs) are promising candidates for stationary energy storage due to their intrinsic safety, low cost, and the abundance of zinc resources. Zinc additionally offers a high theoretical gravimetric capacity of ca 820 mAh g^{-1} and a low redox potential of −0.76 V vs SHE, enabling relatively high operating voltages within the electrochemical stability window of water.

In this work, spent LFP is reutilised as a cathode in AZIBs using environmentally friendly water-soluble binders as alternatives to standard fluorinated systems. Electrochemical delithiation of LFP in Li half-cells was utilised to obtain FP while preserving the olivine framework and conductive carbon coating of the original particles. The resulting FP electrodes were studied in aqueous $ZnSO_4$-based electrolytes to investigate their compatibility with this mild pH system and evaluate their electrochemical behaviour.

Influence of Zn-C-based nucleation layer on the Na metal deposition

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Zero-excess sodium metal batteries (ZESMB) offer higher energy densities and lower production costs compared to sodium-ion batteries. However, their cycle life is limited due to dendrite growth and the formation of dead sodium caused by uneven sodium plaiting/stripping. Sodiophilic elements such as zinc have been identified in the existing literature as effective additives to improve negative electrode performance by lowering the sodium nucleation overpotential through the formation of an irreversible NaZn13 alloy.[1] To minimize this sodium consumption, Zn is often incorporated as nucleation seeds within thin, low-cost carbon-based layers.
In this study, a systematic comparison of impregnation, dry mixing, and magnetron sputter coating was conducted to produce Zn–C composite nucleation layers on aluminum-based negative electrodes. The influence of these preparation methods, as well as the effect of the timing of zinc addition during Zn-C synthesis, on electrode morphology, Zn distribution, and electrochemical performance was evaluated in coin cells using NaNi1/3Fe1/3Mn1/3O2 (NFM) as cathode material. The results show that both particle-level Zn coating by impregnation or dry mixing and electrode surface coating by magnetron sputter coating lead to improved electrochemical performance. However, differences in hard carbon matrix utilization were observed, since the C-matrix of electrodes coated using magnetron sputter coating does not contribute to capacity to the same extent as particle-level Zn coating, which appears to render the C-matrix obsolete for sputter coating. The nano-structurization of the surface is of pivotal significance for homogeneous sodium plaiting.

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Impact of treatment method on delamination process for the maximal recovery rate of cathode powder

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The increasing use of electronic products and electric cars has brought several benefits to human society, but also significantly increased waste batteries. Currently, a large variety of LIBs are used for transportation, most containing graphite as the anode material and lithium-MOx (M = Co, Ni, Mn) as the cathode material. These are widely used because of their high energy density, capacitance, durability, and safety. The recycling process mixes battery materials from different sources, and scarce minerals are recovered from this 'black mass'. These can be further purified using hydrotreatment methods, but these involve chemical steps and require large amounts of energy. Even after purification, the recovered metal components contain impurities, negatively impacting battery electrochemical properties. It would be more economically and environmentally justified to use these recovered materials directly without purification in applications that also decrease CO_2 emissions from processing. Direct utilization of cathodic black mass would be a fast and robust way to use the recovered material.

In this study we will use NCA Batteries (capacity3400mAh). After battery discharging and opening, we obtained cathode sheets, which were used to study impact of the treatment method on delamination process for the maximal recovery rate of cathode powder. Four treatment methods were tested: mechanical, ball milling, ultrasound bath with NMP solvent and thermal treatment. The comparison of these methods will be based on Key Performance Indicators: impurities in the cathodes powders (material characterization with XRD and SEM-EDX) and material loss. The most effective treatment methods are ball milling and thermal treatment.

High intensity magnetic separation for high grade cathode active material separation from black mass

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Lithium-ion battery technology has become the leading solution for energy storage with demand rising due to transport electrification and the transition from fossil fuels. Battery recycling offers a way to alleviate the pressure on raw material supplies. Currently, the most common process includes mechanical pre-treatment to create a marketable black mass fraction containing the battery's active materials, which are then processed through hydrometallurgy to recover valuable metal salts. However, heterogeneous and dynamic nature of black mass requires adaptable processing. High intensity magnetic separation provides a promising approach to enrich the paramagnetic cathode active material (CAM) from black mass, producing a high-grade CAM fraction.

In this study, a high intensity magnetic disc separator operating in dry mode was applied to black mass sample derived from end-of-life NMC532 cells. The process produced a CAM-rich fraction in a single pass, achieving a purity greater than 80% and a recovery rate of 95%. Furthermore, the copper content in the magnetic fraction was reduced to below 0.1%. This method helps also to balance fluctuations in the black mass feed, which may enhance the efficiency of subsequent processing steps. Applying a multi-stage separation process may further increase the CAM purity, making it an attractive feedstock for direct recycling approaches.

High intensity magnetic disc separation offers a promising approach for producing high-quality CAM fractions in dry mode from heterogeneous and dynamic black mass. A single-stage operation can act as a homogenization step before hydrometallurgical treatment, while multi-stage processing may serve as a pre-separation method for direct recycling.

Flotation-based direct-recycling of black mass using sustainable frother reagents

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Direct recycling of end-of-life lithium-ion batteries (LIBs) via froth flotation is gaining traction, but a systematic selection of froth stabilization reagents has been largely overlooked. In response to the global attention on transitioning to more environmentally friendly processes, this study explores sustainable alternatives to conventional frothers. Three frother systems were investigated: hydroxypropyl methyl cellulose (HPMC), a sustainable cellulose-based polymer; methyl isobutyl carbinol (MIBC), a commercially available frother; and a polymer-surfactant (PS) mixture comprising HPMC and MIBC. In flotation experiments with model black mass containing nickel manganese cobalt oxide (NMC) cathode material, the PS-mixture delivered superior performance, achieving 97% overall graphite recovery and 93% separation efficiency. Furthermore, experiments were conducted on model black mass containing ultrafine lithium cobalt oxide (LCO). In the latter case, the use of cellulose-based frothers resulted in entrainment of LCO particles, reducing the purity of graphite in the concentrate. Despite this limitation, the PS-mixture consistently produced faster flotation rates than MIBC across both campaigns. These are promising results indicating that a careful selection of sustainable reagents for LIBs flotation can also provide superior performance than commercial reagents.

Impact of the discharge method on preserving the battery electrode integrity

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The rapid growth in electric vehicle (EV) adoption has sharply increased lithium-ion battery (LIB) demand, driving the urgent need for sustainable recycling strategies. Among all recycling technologies, direct recycling aims to recover electrode materials while maintaining their structural and chemical integrity, making it a promising strategy. A critical preprocessing step in battery recycling is the safe discharge of spent LIBs [1]. In this study, we present the comparative analysis of electrical and electrochemically discharge methods and their impact on the morphology and composition of electrode materials using different characterization techniques. From SEM-EDX, we have observed that there is no morphological degradation at the electrode's surface discharged by the electrochemical discharge method. ICP-OES results showed that the Li-ion content at the negative electrode is higher in the electrical discharge sample than in the electrochemical discharge sample. This might be possible when some Li^+ remains intercalated in graphite during incomplete discharge, or surface passivation or a degraded SEI layer prevents Li^+ from leaving the graphite structure [2]. Our findings demonstrate that, unlike standard electrical discharge, electrochemical discharge preserves both the chemical composition and structural integrity of electrode materials. Additionally, this method proves more effective for processing small-scale and mixed LIB waste.

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A Novel direct recycling of LIbs via sequential magnetic separation and froth flotation

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Direct recycling of lithium-ion batteries (LIBs) aims to recover active electrode materials with preserved structure, chemical composition and functionality. Physical separation is thus a prerequisite: in black mass, cathode and anode particles are intimately mixed and must be isolated with sufficient purity and yield. To facilitate such separation, pyrolysis has been proposed to improve liberation, yet the temperatures required to decompose polyvinylidene fluoride (PVDF) binder have shown to alter the cathode crystal structure and compromise the aim of direct recycling. This work investigates wet high-intensity magnetic separation (WHIMS) combined with froth flotation for simultaneous cathode (NMC) and anode (graphite) recovery from black mass and evaluates non-thermal pretreatments to address ultrafine NMC loss and residual PVDF binder on NMC surfaces. Four WHIMS conditions produced flotation feeds with graphite:NMC ratios ranging from 40:60 to 80:20. Graphite floated fast under all conditions, but NMC co-reported to the froth phase, driven by PVDF-enhanced true flotation as well as entrainment of ultrafine particles. The best combined result upgraded graphite from 36 wt.% in the feed to 80 wt.% at 65% recovery, and NMC from 56 wt.% to 90 wt.% at 78% NMC recovery. Targeted pretreatments addressing residual PVDF binder and ultrafine NMC loss showed promising reductions in NMC contamination of the graphite product. The results demonstrate that thermal pretreatment is not a prerequisite for physically separating NMC black mass, and that combining WHIMS with flotation may yield cathode and anode products of sufficient grade for direct recycling and reintroduction into the LIB production chain.

A novel approach for Li recovery from black mass and lithium slag of spent LIBs

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Lithium is a critical raw material essential for lithium ion batteries (LIBs). The EU Batteries Regulation (EU 2023/1542) establishes mandatory lithium recovery targets for spent LIBs of ≥50% by 2027 and ≥80% by 2031. Lithium can be recovered from black mass (BM) or from lithium slag (LS), a Li containing slag generated during thermal processing of spent LIBs. The lithium contents of BM and LS were approximately 5 wt% and 4.3 wt%, respectively.

Lithium was successfully recovered from BM using sulfuric acid leaching, with optimized temperature, solid to liquid ratio, and acid concentration. In conventional sulfuric acid leaching with H_2O_2, a lithium concentration of 5.9 g/L was achieved in the metal sulfate solution. An innovative alternative approach for lithium recovery was also demonstrated, in which $NiSO_4$ was used as a leaching agent instead of sulfuric acid to extract lithium from NMC811 cathode active material. Lithium yields of up to 92.5% were achieved, with higher nickel content enhancing lithium extraction at 150 °C. Following delithiation, the resulting solid was successfully applied for manganese control during sulfuric acid leaching.

For LS, a soda leaching process was developed that enables integration with primary lithium production. Extraction temperature and Ca/Li ratio were identified as key parameters controlling lithium recovery. Lithium leaching efficiencies exceeding 90% were obtained, with Li concentrations of approximately 10 g/L at a Ca/Li ratio of 1.25. Overall, several effective routes were demonstrated for high yield lithium recovery from spent batteries, enabling lithium precipitation as LiOH or Li_2CO_3 for battery reuse.

Valorisation of battery scrap leach residue as a reductant in nickel slag cleaning

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Recently, great efforts have been made to develop efficient recycling processes for spent lithium-ion batteries. Many processes are based on hydrometallurgical routes, starting with pretreatment followed by leaching. Most of the research on hydrometallurgical recycling focuses on extracting and purifying battery metals present in the leach solution. However, the solid leach residue - rich in graphite, organics, and undissolved metals - receives far less attention.

In our study, four residues from different pretreatment–leaching scenarios (Figure 1), containing 49–85 wt% total carbon and varying proportions of graphite, organic carbon, and metals, were used as reductants in nickel-slag cleaning process. In each experiment, a mixture of industrial Ni slag, 5 wt% Ni concentrate, and 4 wt% leach residue was used as a feed material. Experiments were conducted in an inert atmosphere at 1350 °C for 3 to 30 minutes.

Carbon in the leach residue was found to be an effective reductant for metal oxides from both Ni slag and leach residue. In all samples, the matte phase was formed rapidly and acted as a collector of Ni, Co, Cu and Fe in the process. It was observed that the distribution coefficient of nickel was higher in comparison to cobalt and with higher amount of carbon in the leach residue, higher distribution coefficients of both metals were achieved. These results demonstrate that battery leach residues can function as effective reductants and metal carriers in slag cleaning, offering a pathway to valorise a typically overlooked waste stream while improving overall metal recovery.

Effect of pyrolysis pre-treatment on leaching of industrial lithium iron phosphate-based black mass

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Lithium iron phosphate (LFP)-based battery chemistries have gained significant market share in electric vehicles and large-scale energy storage systems. To meet the recovery targets and promote circularity when these batteries reach end-of-life, recycling strategies must be investigated and optimized. In this work, pyrolysis was investigated as a pre-treatment method for heterogeneous, industrial LFP-based black mass (with Mn, Ni and Co also present) before leaching. The black mass was pyrolyzed at 400, 500 and 600 °C for 60 minutes, after which the samples were leached in 0.5M H_2SO_4 for 60 minutes at 25 °C.

During pyrolysis, the mass losses ranged from 11.9 wt% (400 °C) to 14.9 wt% (600 °C). Leaching of the pyrolyzed samples was carried out in mild conditions to see if the pyrolysis pre-treatment enables efficient leaching using less chemicals and lower energy input. The results showed that the pre-treatment has a clear effect on the leaching behavior of all major elements present in the black mass: an example is shown in Figure 1 for Li. The leaching yield is clearly highest for the sample pyrolyzed at 500 °C, followed by 600 and finally 400 °C samples. At 500 °C, the binder degradation seems to be relatively comprehensive, but the cathode material structure is not significantly affected, unlike at 600 °C. In all cases, the extractions at 60-minute time are higher than for the unpyrolyzed sample. Based on the results, 500 °C is the optimum pyrolysis temperature leading to highest extraction yields of Li, P and Mn.

Direct Regeneration of NMC811 Cathodes with Different State of Health Using a Dual-Function Lithium-Replenishing Coating

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Direct recycling offers a promising route to recover spent lithium-ion battery cathodes while preserving their valuable crystal structure and reducing the energy demand associated with conventional hydrometallurgical and pyrometallurgical processes. However, the regeneration efficiency of Ni-rich layered cathodes strongly depends on their degradation history and state of health, as lithium loss, surface reconstruction, and impedance growth become more severe during cycling. In this work, spent $LiNi_{0.8}Mn_{0.1}Co_{0.1}O_2$ cathodes with different states of health are directly regenerated using a dual-function lithium-replenishing protective coating. The proposed coating acts simultaneously as a local lithium source during thermal regeneration and as a stabilizing surface layer after treatment. This approach is designed to compensate for lithium deficiency, promote restoration of the layered α-$NaFeO_2$ structure, and suppress surface side reactions during subsequent electrochemical cycling. The regenerated materials will be systematically compared as a function of the initial degradation level using structural, morphological, surface chemical, and electrochemical characterization, including X-ray diffraction, electron microscopy, X-ray photoelectron spectroscopy, and charge–discharge testing. Particular attention will be paid to the relationship between the initial state of health, lithium replenishment efficiency, surface reconstruction, and capacity recovery. This study aims to demonstrate that regenerative coatings can provide a versatile strategy to improve the direct recycling of Ni-rich cathodes with varying degradation histories, enabling both structural repair and interfacial stabilization in a single treatment step.

On-site direct recycling of LFP production scrap as local raw material source for European batteries

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As Europe transitions towards battery reliant energy and transport systems, the risk of substituting fossil fuel reliance with new dependencies on external raw material supply chains rises. Battery recycling with reuse of secondary raw materials is therefore critical to build more sustainable and strategically autonomous energy system, yet their implementation into production lines requires further research.

Production scrap from cell manufacturing is currently the main feedstock in battery recycling presenting an immediately available local raw-material source. In this context, the present study investigates on-site direct recycling of lithium iron phosphate (LFP) production scrap using thermal treatment between 200°C to 600°C in air and N2 environments. Techno economic and environmental assessments identified the most promising recycling conditions, which were then implemented in new cells using blends of recycled and virgin LFP (100, 50, and 30wt% recycled material). Studied slurry configurations' material costs and environmental impact were also quantified.

Production scrap recycled at 200°C in air and 400°C in N2 maintain the LFP crystalline structure and surface morphology. In addition, recycling at 200°C in air delivered excellent electrochemical performance at 30 wt% recycled content, while reducing active material costs by 28% compared to pristine materials. Recycling at 400 °C in N_2 preserved high capacity even at 100 wt% recycled content. All recycled slurry configurations also showed reduced environmental impact.

With its assuring electrochemical results and evident cost and environmental advantages, the low-temperature direct recycling process demonstrates potential for industrial use making LFP scrap a promising local resource for the European battery sector.

Towards Direct Recycling of NMC811 Cathode Active Material for Lithium-Ion Batteries

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The increased demand for lithium-ion batteries (LIBs) has amplified the need for sustainable recycling processes to recover critical raw materials like lithium, nickel, and cobalt, and to address the environmental repercussions of inadequate waste disposal. Traditional recycling techniques often destroy the chemical structure of the cathode; however, direct recycling may offer an eco-friendly, cost-effective solution with reduced energy consumption, emissions, waste, and environmental impact by regenerating degraded cathode materials and retaining their functional layered structure. As a promising next-generation cathode due to its high energy density and reduced cobalt content, nickel-rich NMC811 ($LiNi_{0.8}Mn_{0.1}Co_{0.1}O_2$) still lacks well-developed direct recycling strategies.

In this study, a direct recycling approach was investigated to thermally treat degraded cathodes to separate Cathode active material (CAM) from current collectors and to regenerate degraded NMC811 cathodes through a molten eutectic salt relithiation process. The pristine NMC811 was prepared by mixing NMC811 precursor ($Ni_{0.8}Mn_{0.1}Co_{0.1}(OH)_2$) with lithium hydroxide (LiOH) in a 1:1.05 molar ratio to compensate for Li losses during high temperature synthesis at 800 °C for 12 hours in an oxygen-rich tube furnace atmosphere. To emulate the lithium (Li) deficiency observed in end-of-life batteries, simulated aged (SA) NMC811 materials were synthesised. Subsequently, five compositions of SA cathodes with varying Li content ($Li_{0.5}$-$Li_{0.9}$) were synthesised intentionally by reducing the stoichiometric amount of LiOH during synthesis. The composition $Li_{0.7}Ni_{0.8}Mn_{0.1}Co_{0.1}O_2$ was chosen for relithiation. The SA NMC811 (Li=0.7) underwent eutectic salt relithiation at 400 °C for 4 hours using a 3:2 molar mixture of $LiNO_3$ and LiOH to replenish the Li content, followed by annealing at 800 °C to restore the layered crystal structure. X-ray diffraction (XRD) analysis confirmed the recovery of pristine-like structure, while the electrochemical characterisation of coin cells demonstrated enhanced specific capacity (mAh/g) and cycling performance compared to as-prepared SA materials.

The electrochemical performance of pristine NMC811, SA, and relithiated NMC811 was evaluated using galvanostatic cycling. The pristine material exhibited the best performance, with a capacity retention of 86.6% after 100 cycles. In contrast, the SA NMC811 showed negligible capacity and poor efficiency due to inactive cathode structure and severe cation mixing as confirmed by XRD analysis. The relithiated material subsequently recovered its electrochemical performance with a capacity retention of 76.1%. While the discharge capacity and intensity peak ratio (I_{003}/I_{104}) indicated relatively complete restoration, the relithiated samples showed slightly higher polarisation and moderate cation disorder compared to the pristine. Overall, relithiation demonstrated successful structural recovery and enhanced electrochemical performance relative to the SA material, though not fully equivalent to pristine NMC811.

Thermal treatment was done at 600 °C for 45 minutes under two different gas atmospheres: Ar and Ar + 10% O_2. The conditions were selected to account for the degradation temperatures of organic compounds like PVDF (polyvinylidene difluoride) binder and conductive carbon. Different characterisation techniques were used to evaluate the separation effectiveness and the crystal structure of CAM. The Ar + O_2 atmosphere proved superior, achieving cleaner and easier separation of CAM with reduced carbon and PVDF residues, while preventing full phase transition to the unwanted rock salt phase. The off-gas analyser further confirmed the efficiency of this atmosphere, showing higher concentrations of CO and CO_2 in the off gases, indicating more complete decomposition of organic binder and conductive carbon.

This work offers a sustainable alternative to traditional recycling methods and provides actionable insights to enhance recycling efficiency within a circular battery economy.

Thermal Processing of LFP Black Mass for Sustainable Recovery of Lithium and Phosphorus

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Background

As demand for lithium iron phosphate (LFP) batteries grows, developing efficient recycling routes for black mass is critical. This work, conducted within the Re-FLiP project in collaboration with Stena Recycling, Volvo Cars, and Chalmers University of Technology, investigates a dual approach of pyro and hydro processing for the recovery of Lithium (Li) and Phosphorus (P) and valorization of iron (Fe) and graphite.

Methods

The safety and hazardous gas evolution of spent LFP pouch cells were first evaluated using a punch simulator across various temperatures. Subsequently, LFP black mass underwent a two-step thermal treatment. Initial pre-treatment was performed in a muffle furnace at a mild temperature (~500 °C) to decompose organic binders. This was followed by high-temperature smelting in a Tammann furnace at 1600 °C to facilitate the carbothermic reduction and volatilization of key elements Li and P.

Results

Preliminary results indicate high efficiency for gas-phase recovery, with >95% of Li and approximately 60% of P successfully captured in the vapor phase. The remaining P and Fe were recovered as a metallic alloy within the surplus graphite residue. These findings demonstrate that the Re-FLiP concept can effectively partition Li and P from the iron-rich LFP matrix.

Conclusions

This thermal route provides a promising primary separation step for LFP recycling. Ongoing work focuses on further refining the recovered fractions and integrating hydrometallurgical polishing at Chalmers University to valorize the recovered valuable elements as high-purity battery-grade precursors.

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Non-Corrosive Electrochemical Discharge of Lithium-ion Batteries for Safe Recycling Preprocessing

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Efficient electrochemical discharge of LIBs before recycling is essential to avoid short circuits and thermal events during mechanical processing. One of the cost-effective and scalable methods is electrochemical discharge using aqueous inorganic salt solutions. However, this approach has issues such as slow discharge rates, extensive battery casing corrosion when NaCl is used as the salt, and toxic gas emissions [1]. The redox couples in an aqueous medium provide both oxidation and reduction reactions to consume electrons and cause no corrosion on the battery casing; however, in water, there is a possibility for side reactions [2].

To fully avoid battery casing corrosion and to recover the battery active materials, this study explores the organic electrochemical discharge. We used the discharging medium Manganese acetylacetonate salt in propylene carbonate solvent with tetrabutylammonium tetrafluroborate as supporting electrolyte, with a continuous N2 purge to minimize oxygen or moisture in the electrolyte (Fig. 1A). The discharge current is mediated by the redox activity of Mn(acac)3, where oxidation of Mn at the positive electrode and reduction of Mn at the negative electrode generate a current that discharges the LIBs. FTIR and XPS spectroscopic analysis results confirmed no significant solvent decomposition or changes in manganese oxidation states, indicating a stable system. This demonstrates safe and efficient extraction of charges from LIBs in an organic medium.

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More sustainable recycling of Li-ion batteries via novel technologies and use of biodegradable reagents

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Background: The necessity of more environmentally friendly processes for the metal's recovery is nowadays evident due to the significant demand for raw materials. Organic biodegradable solvents represent possible pathway for more sustainable development in the mining and recycling industry.
Results: An early selective recovery of lithium from NMC type battery waste using oxalic acid as a leaching agent was investigated and optimized via modelling. The different solubility of transition metals oxalates in comparison to lithium oxalate was the main driving force to achieve selective separation in the leaching step. The optimal parameters were identified as 60°C, 60 min, 0.6 M oxalic acid, resulting in 99% leaching yield for lithium, while less than 0.5 % of cobalt and nickel, and 1.5% of manganese were leached.
Also, a hydrometallurgical method for lithium iron phosphate (LiFePO4, LFP) battery recycling was tested using tartaric (C4H6O6) and formic (CH2O2) acids. The study demonstrated that both agents extract 100% of lithium. Moreover, the effect of oxidants in preventing the co-dissolution of specific impurities like iron and phosphorus, especially in formic acid solutions, has been demonstrated. The experimental conditions, 100 g/L, 0.5 M CH2O2, 2.5 vol% H2O2, 25°C, and 250 rpm, suppressed the iron and phosphorus leaching by >90%.
Conclusion: A complete lithium extraction has been demonstrated using biodegradable substances. Moreover, lithium recovery via organic acids showed superior selectivity towards inorganic acids, simplifying thus a whole recycling process.

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Towards the recycling of Prussian Blue-based Sodium-ion battery via Hydrometallurgy

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Prussian Blue analogues (PBAs), particularly $Na_2FeFe(CN)_6$, are widely used as cathode materials in sodium-ion batteries (SIB) and are characterised by their cyanide-based framework and mixed-valent Fe chemistry. Despite this distinct chemical composition, recycling approaches specifically addressing the behaviour of PBAs during aqueous processing remain limited. The work presented investigates the chemical pathways relevant to the hydrometallurgical recycling of Prussian Blue–based SIB.
The study focuses on the alkaline decomposition of Prussian White, the reduced cathode phase, under conditions relevant for aqueous recycling. Controlled leaching experiments are carried out to convert the solid framework into soluble sodium ferrocyanide while managing iron solubility and preventing uncontrolled cyanide release. The influence of pH (8–11), temperature (20–50 °C), oxidative conditions, and light exposure on the stability of ferrocyanide species and iron speciation is systematically examined.
A central aspect of the work is the development and validation of quantitative analytical methods for cyanide determination in both solid and liquid phases. Free cyanide and complexed cyanide species are quantified using a combination of electrochemical detection and spectroscopic techniques, including UV–Vis or XRD. These methods provide essential feedback for evaluating leaching efficiency and chemical stability during processing.
Following leaching, dissolved iron and aluminum are selectively removed from solution through controlled pH adjustment and precipitation, enabling purification of the ferrocyanide-containing liquor. Overall, this work provides fundamental chemical and analytical insights into the aqueous processing of PBA-based cathode materials and establishes a basis for safe and controlled recycling of SIBs.

Limiting metal losses during froth flotation following thermochemical optimization for direct recycling of lithium-ion Batteries

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Spent lithium-ion batteries (SLIB) contain critical metals, and their improper disposal brings several environmental and economic concerns. Direct recycling of SLIB via froth flotation has recently gained attention since it separates active materials based by physical means, thus preserving their chemical properties and morphological structure. Keeping the structural integrity of active materials is the fundamental definition of direct recycling and only through this condition can the increased economic returns and reduced environmental impact become plausible. However, froth flotation studies have largely overlooked the potential loss of metals from cathodic species into process water. In this study a Response Surface Methodology (RSM) with a Box–Behnken Design (BBD) was applied to evaluate the integrated effect of flotation water pH, temperature, and solid liquid ratio (S/L) with the objective to minimize the metal dissolution. Model black mass containing NMC 111 cathode particles mixed with graphite were subjected to laboratory scale flotation experiments. It was found that flotation water pH and temperature had no effect on the recovery and grade matrices, whereas an increase in the S/L lead to an increase in the graphite recovery while grade is reduced. The dissolution yield for cathode metal(s) was significantly reduced under the optimized conditions of a pH 10, temperature 8 °C, and a S/L of 120 g/L. The present work demonstrated the influence of thermo-chemical parameters during flotation of SLIB and identify optimized conditions for the efficient use of flotation for direct recycling of SLIB.

Social materiality analysis of lithium-ion batteries and process simulation-based life cycle sustainability assessment framework

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The rapid growth of lithium-ion batteries (LIBs) and their critical role in energy transition have led to increasing interest in assessing their sustainability across the entire life cycle. Previous studies have focused on environmental and economic aspects of LIBs, while the social dimension remains comparatively underexplored. Although the United Nations Environment Programme (UNEP) "Guidelines for Social Life Cycle Assessment of Products and Organizations" (2020) provides methodological support, the application of social life cycle assessment (S-LCA) is still evolving, with inconsistencies across studies, making it difficult to determine which stakeholders and social impact categories should be prioritized in a consistent and justified manner. This research conducted a materiality assessment through a systematic review of state-of-the-art S-LCA studies on LIBs to identify the most relevant and significant social hotspots. The results reveal that worker-related issues are the most prominent, particularly health and safety, forced labor, and child labor, followed by corruption within the society stakeholder category, providing guidance for prioritizing stakeholders and social impacts categories in future LIBs-related S-LCA studies. Furthermore, a comprehensive life cycle sustainability assessment framework integrating process simulation was proposed. Process simulation generates process-specific mass and energy balances data, supporting environmental impacts assessment directly, and through conversion into monetary units, enables the integration of life cycle costing by factorial cost estimation method and database-driven S-LCA, thereby linking all three dimensions of sustainability within a unified framework.
This work was supported by the Business Finland-financed project TOCANEM 2.0 (grant number 5373/31/2023) and by the Mitacs Globalink Research Award (Ref. IT48658).

Solid contaminants from battery black mass reshape lithium carbonate crystallization and solid–liquid separation

Presentation type: Poster · **Theme:** 5. Recycling

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Mechanical pre-treatment of spent lithium-ion batteries carries residues into hydrometallurgical process streams: binder-derived poly(vinylidene fluoride) (PVDF), separator-derived polyethylene (PE), anode graphite, and dissolved fluoride from PVDF and $LiPF_6$ decomposition. These contaminants are unlikely to be fully removed upstream and therefore reach the lithium carbonate precipitation step, yet their effect on lithium recovery remains largely unexplored.

Li_2CO_3 was precipitated from aqueous Li_2SO_4 solutions at 80 °C at controlled polymer loadings (0.01–1.0 wt%), and crystallization kinetics, particle size distribution, filtration behaviour, yield and morphology were evaluated by in situ turbidity monitoring, laser diffraction and microscopy. PVDF markedly modified crystallization: turbidity onset times were shortened and significantly finer particles formed, causing pronounced deterioration of filtration performance at higher loadings. Microscopy showed Li_2CO_3 crystallites nucleating preferentially on PVDF surfaces, forming dense agglomerates rather than the well-defined crystals obtained in polymer-free systems. PE produced similar but substantially weaker effects, without surface-mediated nucleation. Yield remained within 68–80% across all systems. Ongoing work extends the same protocol to anode graphite and dissolved fluoride, individually and combined. Graphite emerges as the dominant contaminant for solid–liquid separation, and the combined graphite–fluoride system behaves non-additively rather than cumulatively; the underlying mechanism, supported by SEM–EDS and XRD.

Across both polymer and inorganic contaminants, precipitation yield is remarkably robust while filterability is not. Contaminant management in black mass flowsheets should therefore be framed as a solid–liquid separation problem.

Scalable processing of LFP cathodes: from lab-scale to roll-to-roll using aqueous slurries

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Background
Lithium iron phosphate (LFP) is a promising cathode material for sustainable lithium-ion batteries due to its inherent safety, low cost, and long cycle life. Conventional cathode manufacturing relies on polyvinylidene fluoride (PVDF) binder material and N-methyl-2-pyrrolidone (NMP) solvent, which raise environmental and economic concerns. Aqueous processing using carboxymethyl cellulose/styrene-butadiene rubber (CMC/SBR) binders offers a more sustainable alternative, although challenges remain in achieving comparable electrochemical performance and scalability with the PVDF binder system.
Results
In this work, LFP cathodes were fabricated using solvent-based (PVDF/NMP) and aqueous (CMC/SBR) slurries via slot-die coating and screen printing at laboratory scale, followed by pilot-scale roll-to-roll (R2R) processing. Optimized aqueous formulations enabled uniform coatings with good adhesion to the aluminium current collector. Electrochemical performance was evaluated in half-cells. Aqueous CMC/SBR cathodes showed lower rate capability than PVDF/NMP cathodes at high C-rates, while exhibiting comparable behavior at lower C-rates (Figure 1 - Rate capability comparison of slot-die and screen-printed LFP cathodes using solvent-based and aqueous formulations).
Screen-printed cathodes performed similarly to slot-die coated cathodes, indicating that the fabrication method did not significantly affect cell performance while enabling patterned electrode architectures. Furthermore, R2R-processed rotary screen-printed aqueous cathodes exhibited comparable rate capability and voltage behavior to laboratory-scale electrodes, confirming successful process scale-up.
Conclusions
Aqueous CMC/SBR-based LFP cathodes provide a scalable and sustainable alternative to PVDF-based binder systems. Combined with the patterning capability of printing and compatibility with R2R printing, this approach shows strong potential for industrial electrode manufacturing.

Hybrid Thin-Film Deposition for Stabilizing Lithium-Metal Interfaces in Solid-State Batteries

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Thin lithium-metal negative electrodes are essential for achieving high energy densities in next-generation solid-state batteries due to their reduced inactive mass and volume [1]. However, the fabrication of stable and uniform lithium thin films, as well as maintaining a robust interface with solid electrolytes, remains highly challenging [2]. These limitations arise from interfacial instability, poor physical contact, and surface heterogeneity, which can lead to non-uniform lithium plating and stripping and ultimately accelerate cell degradation. Here, we demonstrate the fabrication of dense and uniform lithium thin films via pulsed laser deposition (PLD), providing precise control over film thickness and surface morphology. To improve interfacial stability, a hybrid inorganic coating was applied using thin-film deposition techniques to modify the lithium surface. The electrochemical performance of lithium electrodes with uncoated-lithium and different coated-lithium configurations, was evaluated in solid polymer electrolyte-based cells. We identify three key interfacial behaviors: (i) unstable interfaces and rapid cell failure for uncoated lithium, (ii) improved stability with coated electrodes, and (iii) enhanced interfacial stability and reduced polarization for the hybrid-coated system. The modified interfaces showed more controlled lithium deposition behavior and reduced interfacial degradation, highlighting the importance of surface engineering for improving lithium-metal stability in solid-state battery configurations.

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Roll-to-Roll Manufacturing and Inline Quality Control of Solid-State Battery Components on Pilot-Scale Production Lines

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Abstract

The industrialization of solid-state batteries (SSBs) requires manufacturing technologies that enable large-area processing and reproducible quality control. Within the SOLiD project, we have demonstrated pilot-scale roll-to-roll (R2R) manufacturing processes for both cathode composites and solid polymer electrolyte layers, supported by advanced inline characterization.

A solvent-free dry extrusion route was developed for NMC811-based cathode composites utilizing a thermoplastic polymer-electrolyte binder. Following rheological optimization and laboratory-scale validation, the process was transferred to continuous pilot-scale production, including compounding, extrusion, calendering and lamination. Continuous cathode rolls with controlled thickness and homogeneous material distribution were successfully manufactured, demonstrating the suitability of extrusion-based processing for scalable SSB electrode production.

In parallel, a UV-curable separator solid polymer electrolyte (SSPE) was formulated for R2R slot-die coating. Ink rheology was tailored to enable thin and uniform coatings compatible with multilayer battery architectures. The coating process was implemented on VTT's pilot coating infrastructure, enabling systematic investigation of process parameters, coating quality and scalability.

A key contribution of the work is the integration of inline sensing technologies directly into the pilot manufacturing environment. Electrochemical impedance spectroscopy and a high-resolution line-scan camera system were integrated into the R2R coating line to provide real-time information on coating quality, defect formation and layer uniformity. The collected process data are being utilized for feedback-loop control, artificial intelligence-based process optimization and digital twin development, targeting future zero-defect battery manufacturing.

The presented results demonstrate how pilot-scale R2R manufacturing combined with inline quality control can accelerate the transition of solid-state battery technologies from laboratory development towards industrial implementation.

Keywords: solid-state batteries, roll-to-roll manufacturing, dry extrusion, slot-die coating, inline characterization.

From full-cell voltage to open circuit potential: A non-invasive automated parametrization workflow

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Accurate electrochemical battery model parameters are crucial for model accuracy and performance. However, obtaining accurate parameter values can become a long and expensive process involving multiple estimation steps.

This work aims to identify the battery electrode materials, their content ratios and thermodynamic properties using non-invasive means. This is done by performing a differential capacity analysis on full-cell open circuit voltage (OCV) profiles. Electrode open circuit potentials are reconstructed using multiple-site multiple-reaction models. By constructing a lumped parameter single particle model, it becomes compatible with voltage and current as only input-output data. The single particle model is used for parameter optimization and validation using synthetic and experimental OCV data. Synthetic data generation is also utilized for optimum experiment protocol design to maximize parameter identifiability and accuracy for specific battery cell design and application. The whole parameter estimation workflow and experiment design is automated using a workflow manager.

Automated electrochemical model thermodynamic parameter estimation workflow with experiment design aims to minimize resource usage for experiments, by delivering optimum non-invasive experimental protocols for specific chemistry and application. The workflow works as fast “plug and play” tool that accelerates first steps of electrochemical model parameterization by automating the process, saving time and making estimation process repeatable.

All in all, proposed workflow automates the thermodynamic parametrization pipeline. Going from electrode identification to experiment protocol optimization. Delivering a fast, repeatable, and non-invasive tool that accelerates electrochemical battery model development.

Toward Electrode-Resolved Parasitic Reaction Enthalpy Analysis for Early Detection of Aging in Lithium-Ion Batteries

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Parasitic side reactions strongly influence the long-term lifetime of battery cells, contributing to heat generation, active lithium loss, and capacity fade. Understanding these reactions is essential for designing cells with improved longevity. Of equal importance is whether degradation is dominated by the same reaction pathways throughout cell lifetime or shifts as the cell ages. Isothermal microcalorimetry (IMC) has been utilised successfully for operando detection of parasitic reactions, paired with electrochemical testing and correlated with lifetime behaviour. However, a key limitation of current IMC approaches is the difficulty in resolving the nature of parasitic reactions occurring. Some efforts have addressed this to varying degrees of success [Krause et al., 2012; Glazier et al., 2018], and this work aims to develop this further.

This work presents a preliminary experimental framework to separate electrode-specific parasitic reaction enthalpies using IMC combined with ultra-high precision coulometry (UHPC). Rather than relying on full-cell measurements, parasitic thermochemistry is resolved using reference configurations that isolate electrode behaviour, including symmetric cells, separating SEI-dominated reactions at the negative electrode from electrolyte oxidation at the high-voltage positive electrode. Apparent parasitic reaction enthalpies are quantified using voltage-hold experiments and narrow voltage-window cycling. Measurements are performed in low- and high-voltage regimes to distinguish anode- and cathode-dominated processes, and compared with reference cells to evaluate consistency with literature reports of net endothermic full-cell behaviour at high voltages. This methodology provides a basis for early detection of accelerated ageing, tracking of electrolyte changes during ageing, and improved understanding of electrode-specific degradation pathways in lithium-ion batteries.

Understanding Cathode- driven Degradation in LFP/Graphite Battery Cells.

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Graphite/LFP cells have seen enormous use in EVs and BESSs hence it's important to understand how and why these batteries degrade quicker than expected. Although, having strong P-O covalent bonds and no oxygen release below thermal runaway, LFP has poor high temperature lifetime performance. Historically, anode side has been studied with regards to SEI structure, Fe deposition and electrolyte optimization, but less emphasis has been placed on how cathode interacts with the anode and consequently its effect on capacity loss and impedance evolution.

This work presents a controlled study to disentangle LFP cathode degradation mechanisms by comparing cycling, storage, and cathode-only 'pouch bag' experiments. Given the accelerated timeline, the research focuses on streamlined diagnostics at elevated temperatures across varying electrolyte formulations. The study quantifies degradation through these key metrics: cathode-specific capacity loss, evolution of cathode and anode impedance, gas evolution, and parasitic heat generation. By isolating cathode behaviour, this research provides a focused mechanistic map of LFP degradation to inform lifetime optimization.

Calendar and cycle aging induced changes in electrolyte and composition of gases generated will give additional but valuable insights into dominant degradation modes. At the material level, post-mortem SEM and XRD will track particle cracking, impurity/antisite defects, and phase distribution under high-rate and high-temperature stress.

Overall, the study aims to construct a mechanistic map of LFP cathode degradation pathways and quantify their distinct contributions to capacity fade and impedance growth, providing guidelines for extending AG/LFP lifetime.

Remaining useful life estimation with electrochemical physics-informed neural networks

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Background

Predicting battery degradation trajectories to estimate remaining useful Life (RUL) is an important practice in regards to safety, battery operation and cost. RUL is a monotonic decreasing function of a battery's decreasing State of Health (SoH), and depends on a multitude of degradation modes related to battery operation, external influences, battery chemistry and individual cell-, pack and module variations. Data-driven and physics/modelling-based methods are popular in RUL prediction, with hybrid methods gaining popularity in recent years. Physics-based neural networks (PINNs) have emerged as a promising, accurate and flexible method for RUL estimation when physical details or battery models exist, with several potential advantages over for instance convolutional- or transformer models.

Results

We have implemented a PINN for predicting RUL based on anodic solid-electrolyte interface (SEI) growth. The physics is represented by an electrochemical Butler-Volmer model for computing the SEI current, which is used to regularize the neural network. The PINN was initially trained on lab cycling data, and the parameters transferred to a long short-term memory (LSTM) model for predicting the degradation trajectory and subsequently the RUL based on SoH time series data. The work has been performed as part of the EU HORIZON Project BatMax.

Conclusions

Our results demonstrate several aspects of what makes PINN battery modelling attractive, including parameter discovery, good results with noisy data and few datapoints, and ease of implementation, running and training. Future work would include improving PINN accuracy and performance through fine-tuning, or extend the electrochemical model.

Dynamic internal resistance of lithium-ion batteries during real fast charging at different temperatures

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Fast charging is essential for lithium-ion batteries, particularly in electric vehicle applications, but it introduces complex behavior that is not fully captured by conventional characterization methods. In particular, internal resistance is not constant and varies with state of charge (SOC), temperature, and operating conditions.

This study investigates the resistance of a lithium-ion cell during real fast charging under constant current–constant voltage (CC–CV) conditions. Using measured current and voltage data, together with open-circuit voltage (OCV) information, the resistance is estimated throughout the charging process.

The analysis examines the variation of DC internal resistance (DCIR) at different temperatures and evaluates the effect of ambient temperature on DCIR under fast charging conditions. The importance of DCIR for battery thermal behavior is also highlighted, as it directly influences heat generation during high-rate charging.

The results show that resistance evolves continuously during charging and differs between the constant current and constant voltage phases, with a clear dependence on temperature. As an extension of this work, a comparison between experimentally derived DCIR and estimates from equivalent circuit models (ECMs) based on HPPC data can be explored.

Battery module condition assessment using constant-current cycling and electrochemical simulation

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Assessing the condition of lithium-ion batteries is particularly challenging at the module level, where cell-to-cell asymmetries may remain hidden in aggregate measurements. This paper presents a measurement–simulation based approach for battery module condition assessment using a simple constant-current test cycle. Experimentally measured voltage responses are compared with results obtained from a physics-based electrochemical simulation model, and the discrepancies are used to analyze battery aging and cell-level differences. The method is demonstrated using a three-cell series-connected lithium-ion pouch cell module without active cell balancing. The simulation framework is based on the LIONSIMBA model [1].

The results show that the proposed approach is capable of reproducing the overall voltage behavior of the module under a dynamic constant-current profile with good qualitative agreement. Systematic optimization of structural and aging-related parameters enables identification of cell-specific differences within the module, revealing asymmetrical aging behavior that is not directly observable from aggregate measurements alone. In particular, variations in effective internal resistance and capacity between cells can be detected through model–measurement mismatch analysis.

However, the study also highlights limitations in quantitative accuracy, especially in the estimation of state-of-charge and thermal behavior, indicating the need for further model refinement and validation. Despite these limitations, the approach provides a scalable and non-destructive framework for module-level diagnostics of lithium-ion batteries under limited measurement conditions.

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End-of-life gassing and electrochemical degassing in aged Li-ion cells

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One known safety hazard in Li-ion batteries is gas evolution, as it can lead to cell pressure build-up, with concomitant expansion, venting or bursting. Studies on gassing in Li-ion batteries have focused on gas evolution during formation cycling or under extreme conditions (e.g., abuse tests, thermal runaway). Reports on gas evolution under "normal" operation or during storage are scarce.

Here, we report on observations of significant gassing in large-format pouch cells (>60 Ah), from a renowned Li-ion cell manufacturer, during end-of-life (EoL) storage at a supposedly ideal storage temperature (5 °C), as well as on the possibility to remove the evolved gasses through electrochemical degassing.

In cells cycled to EoL at 60-80% remaining capacity (SoH), we initially observed ≤50% solid thickness increase for some of the cells, without gassing. More than a third of these cells then evolved significant amounts of gas during EoL storage at 5 °C. Gas analysis by GC-MS revealed that >95% of the gas was comprised of H_2, CH_4 and C_2H_6, with H_2 being the largest contributor. Small amounts of electrolyte solvents (EMC and DMC) were also found. Notably, CO and CO_2 levels were found to be below 1%. Correlations between the cell thickness increases, SoH and the methane:hydrogen ratios were observed. During careful cycling of the gassed cells, to check their functionality and remaining capacity, we observed that under specific conditions it was possible to electrochemically consume the evolved gasses within the cell.

Streaming battery management data via ethernet with foxBMS for model validation while preserving safety-critical functions.

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To enhance accessibility for a broad community of developers and users, Fraunhofer IISB develops the open-source battery management system platform foxBMS. Both the hardware design and software are open-source and freely available, enabling academic research and serving as a development frame-work for industrial applications worldwide, while celebrating the 10th anniversary of foxBMS in 2025.

This poster presents a communication architecture for the open-source battery management system foxBMS designed to support scientific research on advanced estimation and control algorithms. To enable model validation on external platforms, the safety critical communication required for core BMS functions (cell protection, diagnostics) is separated from non critical high bandwidth data streams intended for model validation and algorithm development (SOX estimation).

The baseline foxBMS platform uses a CAN-based communication layer to guarantee real-time, deterministic behavior for safety-critical tasks. To enable richer observability and data logging, a parallel Ethernet-based communication path dedicated to non-critical data with significantly increased throughput is added. The proposed architecture allows external tools to access detailed measurement and internal state data in real time without interfering with critical BMS functions. The evaluation comprises the impact of the additional communication channel using hardware-in-the-loop experiments and task runtime measurements. Results show that Ethernet data streaming does not compromise timing constraints or safety mechanisms on the main CAN-based control path. The presented approach lowers the barrier for integrating and validating novel battery models and estimators on foxBMS.

Battery Core Temperature Monitoring Using Impedance-Based Data-Driven Models

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The worldwide transition toward electric vehicles and renewable energy technologies has driven rapid progress in battery technology. As requirements for higher performance and improved safety continue to grow, accurate monitoring of battery conditions—especially internal temperature—has become increasingly important. Precise monitoring of battery temperature is essential for maintaining safety and optimal performance, especially given the shortcomings of conventional sensors that only capture surface temperature. This work introduces a novel method that employs Electrochemical Impedance Spectroscopy (EIS) in combination with Machine Learning (ML) to estimate the internal battery temperature. After data collection and preprocessing, several ML models were trained, with hyperparameters optimized using nested Randomized Search CV to obtain unbiased performance evaluation. The Random Forest model delivered the highest accuracy, achieving Root Mean Square Error (RMSE) of approximately 3.88 °C. To improve model interpretability, feature analysis indicated that the imaginary part of the impedance at certain frequencies plays a dominant role in temperature prediction. Overall, the findings demonstrate that data-driven EIS analysis offers a promising non-invasive alternative to surface temperature sensors, supporting the development of more advanced battery management systems (BMS).

A data-centric framework for probabilistic state of health assessment using large scale battery cycling data

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Modern battery systems generate large volumes of cycling data during laboratory testing and in-field operation, characterized by partial cycling, variable operating conditions, and heterogeneous test protocols. While such datasets contain valuable information on degradation behavior, their scale and complexity complicate systematic analysis and reliable state-of-health (SOH) assessment. In practice, SOH is commonly reported as a deterministic indicator, despite substantial uncertainty arising from operational variability and incomplete degradation observability.

In this work, we present a data-centric framework that orchestrates the full pipeline from raw cycling data to probabilistic SOH estimation. The framework integrates cellpy as a standardized interface for ingesting and preprocessing large scale laboratory and field data from standard test systems. These processed data streams are organized within ML-Batt-TOOL, an open machine-learning toolbox designed to support feature extraction, dataset assembly, and model interfacing through a unified, model-ready dataframe.

Within ML-Batt-TOOL, time based summary features can be constructed over configurable windows to capture operational exposure, degradation signatures, and usage induced variability, without requiring complete charge–discharge cycles. These features are used within uncertainty aware machine learning models to produce probabilistic estimates of SOH and remaining useful life, enabling battery health to be interpreted as a risk based prediction problem rather than a single point estimate.

By combining scalable data orchestration, standardized preprocessing, and probabilistic modelling, the proposed framework enables robust analysis of large, heterogeneous battery datasets and supports risk informed diagnostics for both laboratory evaluation and real world operation. Future extensions will incorporate physics based constraints to further enhance robustness and interpretability.

SOC-resolved short current interruption fingerprints for aging-history-aware lithium-ion battery diagnostics

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Capacity-based SOH reduces lithium-ion battery aging to a single scalar and can obscure path-dependent differences between cells with similar remaining capacity [1]. This work asks whether a standardized current-interruption (CI) response, although far from equilibrium, can serve as a SOC-resolved diagnostic fingerprint for aging-history-aware assessment.

During 0.5 C CC-charging, 70 interruptions were applied from 1-70% SOC at 1% SOC spacing, each lasting 3 s. The dataset comprises 46 cells with identical CI procedures within Reference Performance Tests (RPTs) performed at 25 °C but deliberately different aging histories: matched 3×3 aging matrices of charge rate (0.3/0.7/1C) and DoD (30/70/100%) aged at 25 or 10 °C, five additional test cells for each matrix with varied cycling parameters between RPTs, and 100% DoD charge–charge/charge–rest pulse aging at 0.3–0.8C average charge rates with matched CC-CV controls. Amplitude-, time-scale-, and shape-based apparent relaxation descriptors are organized into SOC-resolved maps to separate health-sensitive regions from aging-history-sensitive regions. The novelty lies in preserving an identical diagnostic protocol while deliberately varying aging history, so that same-SOH comparisons can distinguish capacity fade from path-dependent transient signatures. Selected EIS measurements at matched SOCs provide limited impedance-related anchoring [2].

This study reframes short CI from a SOH-regression input into an interpretable probe of hidden aging-history information. The expected outcome is a SOC-window information map that identifies regions associated with general health loss, C-rate/DoD stress, low-temperature aging history, and charging-waveform effects, thereby guiding sparse CI protocols for service diagnostics.

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Technical language processing (TLP) framework for digital battery passport (DBP) and battery predictions

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We introduce the first digital battery passport (DBP) dataset (BatteryPass-12K) and a novel technical language processing (TLP) framework (Fig. 1) for battery predictions. A DBP is an electronic record of the features and history of a battery.1 The TLP framework combines the capabilities of artificial intelligence (AI) agents, large language models (LLMs), and optimized hard and soft prompts. The contributions of our work include (1) introduction of a novel task of DBP or DPP classification with the binary labels of conformant or nonconformant, (2) introduction of the first (synthetic) dataset with 12,000 balanced samples, generated from real pilot samples using ChatGPT5.1 Thinking, and (3) the TLP framework for battery predictions. This is important in view of the EU battery regulation for 2027 to protect the environment and ensure traceability and transparency along the entire battery value chain.

Furthermore, accurately estimating battery state in extreme temperatures is one of the challenges in the battery domain and the TLP framework aims to address this. The electronic record of the entire life cycle of various features of a battery, provided by the DBP, or battery management system (BMS) is useful within the framework for data-driven solutions. It involves a battery-agnostic model context protocol (MCP) AI agent that can connect to external tools and provides soft prompts (continuous feature vectors learned by prompt-tuning) combined with optimized hard prompts (plain text inputs enhanced with gradient-based optimization). The combination is then supplied as input to a capable multimodal LLM for relevant TLP task predictions.

Degradation and modeling of large-format NMC batteries in maritime application

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The maritime transportation industry is expected to see an increased number of larger electric ferries, due to the developments in battery technology, charging infrastructure, and customer base. While the amount of battery research has increased over the past years, there is a gap in investigating lithium-ion (Li-ion) batteries aged using maritime cycles. A multi-stage aging study is conducted for 64Ah LiNi0.5Mn0.3Co0.2O2 (NMC532) based cells, investigating the effects of (i) maritime load cycle, (ii) charge rate, and (iii) periodic change to depth of discharge (DoD). Cells are cycled under semi-controlled temperature with cell surface temperature measured at 21 ± 3 ◦C, using a constant-current constant-voltage (CC–CV) charging protocol across a voltage window of 3.0-4.2 V. Cells are charged with one of three investigated charge rates: 0.5 C, 0.75 C, and 1 C. Discharge depth alternates between 80% DoD and 100% DoD every 400 cycles of maritime cycling. Reference performance tests including rate capability tests, pulse tests, and open circuit voltage tests are conducted in between cycling the cells to measure capacity, internal resistance, and state-of-health. Preliminary results after 800 cycles reveal minimal capacity fade difference for low current discharge (0.75C ≥) in cells charged at 0.5 C, 0.75 C and 1 C and discharged at 80% DoD. These results suggest that, under maritime-representative cycling and moderate discharge rates, increasing charge rate up to 1C may not materially accelerate capacity loss if DoD is 80%. Ongoing work quantifies resistance growth, evaluates higher discharge rates, and conducts post-mortem studies to characterize aging mechanisms.

A Modular Framework for Battery Energy Storage in All-Electric Ships

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This study investigates advanced battery energy storage systems (BESS) for fully electric ships, with emphasis on scalability, modularity, and efficient energy management. The goal is to develop solutions that meet diverse operational requirements while ensuring safety, cost-effectiveness, and lifecycle adaptability. Electric vessels face challenges related to variable load demand, strict maritime regulations, and constraints on space, weight, and maintenance.

To address these challenges, this work proposes a conceptual design framework for modular battery systems tailored to maritime electrification. The approach is based on standardized and reconfigurable building blocks that enable flexible adaptation to different vessel types, mission profiles, and installation constraints. Virtual design and simulation tools are employed to systematically evaluate alternative BESS configurations with respect to key performance metrics, including size, mass, power and energy capability, thermal behavior, and lifetime performance. The framework incorporates computationally efficient electro-thermal battery models alongside advanced battery management functionalities, such as state estimation, health monitoring, and lifetime prediction. The proposed modular scheme is validated through hardware-in-the-loop testing on a MATLAB-Simulink Speedgoat platform.

The study also introduces advanced thermal management strategies, particularly focusing on recovering and using waste heat generated by battery losses, enabling improved integration with overall ship energy systems. The main contribution of this work lies in the integration of scalable modular design, intelligent battery management, waste-heat-aware thermal control, and validation-oriented methodologies, supported by regulatory considerations and system integration guidelines specific to fully electric ship applications. The effectiveness of the thermal management and waste-heat utilization concepts is further assessed through software-in-the-loop validation.

Techno-Economic Analysis and Hybridization Impact of a Battery–Supercapacitor HESS for Grid Stabilization Applications

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Integrating renewable energy sources and rising electric vehicle (EV) use challenge power system stability by reducing inertia and causing greater frequency fluctuations. Energy storage systems are vital for future grids. Li-ion batteries (LiBs) deliver high energy density for sustained use but lack power density and degrade quickly under frequent cycling. Supercapacitors (SCs) offer rapid responses and high power density, yet have low energy density and higher self-discharge rates. Considering these challenges, this paper presents a comprehensive techno-economic analysis and hybridization impact assessment of LiBs and SCs within a hybrid energy storage system (HESS) designed for grid stabilization and EV applications. The study aims to quantify the effects of hybridization on key factors, including CAPEX, OPEX, physical size, weight, operational lifetime, and sustainability. The investigated system comprises a 40kW HESS, integrating a 30kW/150kWh lithium-iron-phosphate (LFP) LiB with a 10kW SC. A fully active HESS topology is employed, enabling independent control of the LiB and SC through bidirectional DC/DC converters. In addition, a power management strategy is implemented to coordinate power sharing, regulate the DC-bus voltage, and divert high-frequency current components to SC in order to mitigate LiB stress. Simulations under variable RES generation demonstrate enhanced dynamic power support, sub-10ms response for fast frequency responses, and reduced LiB degradation under high cycling. Although hybridization increases energy-normalized CAPEX, it has little effect on power-normalized CAPEX, making the HESS cost-effective for power-constrained, high-cycle applications. These findings are further validated for a PV–wind-based grid-independent microgrid using a model-in-the-loop implementation on a Speedgoat® real-time platform.

Fire forensic analysis of lithium-ion batteries

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When a Li-ion battery burns, it is a result of a series of chemical and physical events inside the battery including; melting of the separator creating inner short circuits, reactions between electrolyte and electrodes, cathode material decomposition, and melting of aluminum metal parts. These steps are part of the so-called thermal runaway (TR) which causes rapid temperature rises and, in many cases, fires, and explosions. Thermal runaway occurs irrespectively of whether the heat is created by the cell itself because of an internal short circuit (causal cell), or if an external fire heats the cell (victim cell). Thus, distinguishing the two cases in a post-fire scenario is difficult.

This study seeks to develop a forensic methodology to determine the batteries' role in a fire from a forensic perspective. X-ray computed tomography (X-ray CT) is used to gain three-dimensionally resolved data of the batteries of its internal damage and heat fingerprint. X-ray CT is supplemented with other methods from materials science such as elemental mapping via fluorescence and diffraction.

Literature suggests several potential distinguishing features, such as bowing of the negative end, the degree of damage and location of damage (inner vs. outer layers) to the electrode winding etc. However, there is no agreement of which feature is assigned to what case (cause or victim). Thus, many batteries will be burned under controlled conditions and analyzed thoroughly.