Programme & Book of abstracts for BATTERY 2030+ Annual Conference 2023







Annual Conference 2023 PROGRAMME May 9 – Day 1

09:00 - 09:30	Registration and Coffee + putting up posters	
Moderator:	Philippe Jacques, BATTERY 2030+, EMIRI	
09:30 - 09:40	Welcome by Dean of Science	Anna Qvarnström, Uppsala University
09:40 - 09:50	Welcome by the European Commission	Aymard de Touzalin, DG CNECT
09:50 - 10:00	Swedish batteries and the European perspective	Greger Ledung, Swedish Energy Agency and Swedish delegate in NRCG
10:00 - 10:15	BATTERY 2030+ - some golden nuggets	Kristina Edström, BATTERY 2030+, Uppsala University
10:15 – 10:30	Charging Forward: Role of Batteries Europe and BEPA in Mobilizing European Battery R&I Community	Bozorg Khanbaei, BEPA Estibaliz Crespo, Batteries Europe, CICenergigune
10:30 - 10:45	The EIC hands-on approach for technological innovation within batteries	Olivier Dahon, 12 EIC Pathfinder Open
10:45 - 11:00	Coffee break	
11:00 – 11:45	New spectroscopic approaches to study batteries: intercalation mechanisms, fast charging, and long-term degradation mechanisms	Clare Grey, Cambridge University
11:45 – 12:15	Accelerating research by reinventing the way we do research	Tejs Vegge, BIG-MAP, Technical University of Denmark
12:15 - 13:30	Lunch break and poster session	
13:30 - 14:00	Material Development for the growth of a new Swedish industry producing the greenest batteries in the world	Maria Åstrand, Northvolt AB
14:00 - 15:30	Smart functionalities: Sensing – Scientific outloo	bk and technical results
14:00 - 14:40	Battery optical sensing: from concepts to applications	Jean-Marie Tarascon, Collège de France (CNRS)
	SPARTACUS overview - How to make batteries smart by optimized sensor technologies	Gerhard Domann, Fraunhofer
14:40 – 15:30	SENSIBAT overview - Cell-integrated Sensing functionalities for smart battery systems with improved performance and safety	Iñigo Gandiaga, IKERLAN
	INSTABAT overview – Smart battery from sensing to BMS	Olivier Raccurt, CEA
15:30 - 16:00	Coffee break	







16:00 - 16:05	Introduction Young Scientists	Silvia Bodoardo, BATTERY 2030+, POLITO
16:05 – 17:00	Young Scientist presentations, 10 min each	Moderators: Guiomar Hernandez and Leiting Zhang, Uppsala University
	Dynamic disproportionation and oxygen redox in lithium nickel oxide	Andrey Poletayev, University of Oxford and The Faraday Institution, UK
	An evaluation of the barriers faced by various stakeholders in the EV battery value chain: can the law and policy in the European Union facilitate the transition to a sustainable circular economy?	King Men Teoh, University of Oslo
	Application of organic cathodes for rechargeable multivalent batteries	Jan Bitenc, University of Ljubljana and ALISTORE-European Research Institute
	Operando ultrasonic signal evaluation for a lithium-ion battery	Xia Zeng, Battery Innovation Center, MOBI Research Center, Vrije Universiteit Brussel
	Ethylene carbonate reaction pathways and their respective contributions to the solid electrolyte interphase in Li-ion	Robin Lundström, Uppsala University
17:00 - 17:15	Group photo	
17:15 - 19:00	Poster session and refreshments	









Annual Conference 2023 PROGRAMME May 10 – Day 2

Moderator:	Thore Sekkenes, EBA250		
08:30 - 09:00	A non-academic perspective on applied battery research	Matthew Lacey, Scania	
09:00 - 09:10	Sustainable Battery Metals	Kenneth Ekman, Fortum	
09:10 - 09:20	What could you do with Single Ion Monomers & Polymers	Cédric Loubat, Specific Polymers	
09:20 - 09:30	Design considerations for commercial Sodium-Ion batteries	Ronnie Mogensen, ALTRIS	
09:30 – 09:40	From CoinPower Cells to High-Performance Round Cells – Transferring Know-How in the Development of Different Battery Types	Stefan Koller, VARTA innovation	
09:40 - 10:00	Panel discussion with the companies		
10:00 - 10:30	Coffee break and poster session		
10:30 - 12:00	Smart functionalities: Self-healing – Scientific outlook and technical results		
10:30 - 10:50	Success stories: HIDDEN Success stories: BAT4EVER	Marja Vilkman, VTT K. Burak Dermanci, VUB	
10:50 - 12:00	Characterization and BMS Integration Modelling (atomistic, macrolevel)	Moderators: Marja Vilkman, VTT and K. Burak Dermanci, Battery Innovation Centre at MOBI-Vrije Universiteit Brussel	
	Next-gen battery management systems to support 2030+: highlights from HIDDEN and SPARTACUS	Claudio Brivio, CSEM SA	
	In-situ study of NMC core-shell particles as cathode materials in Li-ion batteries	Javier García-Alonso, Universidad Complutense de Madrid	
	Quantum Chemical Investigation of Thermotropic Ionic Liquid Crystals for Self-Healing Batteries, HIDDEN	Erin Makara, VTT	
	Multiphysics modelling of BAT4EVER cells: from parameters to 1D isothermal models, BAT4EVER	K. Burak Dermanci, Battery Innovation Centre at MOBI-Vrije Universiteit Brussel	
12:00 - 13:00	Lunch and poster session		







	Young Scientist presentations	Moderators: Guiomar Hernandez and Leiting Zhang, Uppsala University
	New, faster, better, and beyond	Helge S. Stein, Helmholtz Institute Ulm and Karlsruhe Institute of Technology
13:00 – 14:00	Stress-driven propagation of lithium plating in commercial batteries	Alexander J. Smith, KTH Royal Institute of Technology
	Using a reference electrode inside Li-ion cell to study the impact of the protocol on aging mechanisms	Alexia Bichon, University of Grenoble Alpes, CEA
	Deciphering Li deposition and SEI with cryo-EM and cryo- ET	Yaolin Xu, Helmholtz-Zentrum Berlin für Materialien und Energie (HZB)
	Complete and Selective recovery of lithium from EV lithium-ion batteries using oxalic acid as a leaching agent	Lea Rouquette, Chalmers University of Technology
14:00 - 15:00	BATTERY 2030+ in the future	
14:00 - 14:10	PHOENIX project	K. Burak Dermanci, Battery Innovation Centre at MOBI-Vrije Universiteit Brussel
14:10 - 14:20	SALAMANDER – A smart, self-healing battery built for a sustainable economy	Samson Yuxiu Lai, Institutt For Energiteknikk (IFE)
14:20 - 14:30	OPERA: Development of operando techniques and multiscale modelling to face the zero-excess solid-state battery challenge	Celia Polop Jorda, Autonomous University of Madrid
14:30 - 14:40	UltraBat - Capturing Ultrafast Electron and Ion Dynamics in Batteries	Martin Meedom Nielsen, Techncal University of Denmark (DTU)
14:40 – 14:50	OPINCHARGE project: goals and expected outcomes	Santhana Eswara Moorthy, Luxembourg Institute of Science and Technology (LIST)
14:50 – 15:00	HealingBat project	Stefan Palzer, Technical University Dortmunt
15:00 - 15:15	Coffee break	
15:15 – 16:00	Panel discussion: The continues development of the European Battery Ecosystem	Moderator: Philippe Jacques, EMIRI Leiting Zhang, Uppsala University Bozorg Khanbaei, BEPA Estibaliz Crespo, Batteries Europe Kristina Edström, BATTERY 2030+ Ilka von Dalwigk, EBA250
16:00 - 16:15	Summary and poster award	







Oral Presentations Young Scientists





Dynamic disproportionation and oxygen redox in lithium nickel oxide.

<u>Andrey D. Poletayev</u>^{1,2}, Robert J. Green³, Robert House^{1,2}, Benjamin J. Morgan^{2,4}, M. Saiful Islam^{1,2,4}. ¹Department of Materials, Univ. of Oxford, Oxford, UK ² The Faraday Institution, Harwell Science and Innovation Campus, Didcot, UK ³ Department of Physics and Engineering Physics, Univ. of Saskatchewan, Saskatoon SK, Canada ⁴ Department of Chemistry, Univ. of Bath, Bath, UK

Layered lithium nickel oxide LiNiO₂ represents the end-member of industry-leading lithium-ion battery cathodes, Li(NiMnCo)O₂. The properties of LiNiO₂ (LNO) are responsible for much of the degradation of such cathodes, especially during high-voltage operation above 4.2 V, presenting an opportunity to improve their energy density by extending the operating voltage window. Here we focus first on the computational and experimental understanding of pristine LNO and its presumed delithiated state, layered NiO₂. LNO possesses several unusual properties: (1) gradual lattice distortions rather than abrupt phase transitions upon cooling, (2) gradual changes to vibrational spectra upon cooling, (3) heat-activated electronic conductivity with a variable activation energy, (4) temperature-dependent NiO₆ distortions, and (5) ubiquitous antisite defects.

We present a comprehensive model reconciling these observations. The nickel ions in LNO find themselves in a mixture of three spin states (S = 1, $\frac{1}{2}$, and 0), reminiscent of formal charge states +2, +3, and +4. The concentration of each specie approaches 1/3 at cryogenic temperatures, reminiscent of LiNi_{1/3}Co_{1/3}Mn_{1/3}O₂, but $S = \frac{1}{2}$ becomes progressively dominant towards elevated temperatures. The antiferromagnetic coupling of S = 1nickels across the Ni–O–Ni motif further stabilizes antisite defects, leading to a negligible defect formation energy at the conditions of synthesis. This model explains the gradual variation of the physical properties of LNO across temperatures [1]. Since small variations in the level of theory lead to substantial changes in the predicted behavior and its temperature dependence, we verify computational predictions experimentally. Resonant inelastic x-ray scattering (RIXS) at the nickel L-edge and temperature-resolved bulk-sensitive x-ray absorption spectra at the nickel L-edge confirm first-principles predictions and offer a path towards Ni species identification.

We extend our model to consider the stability of delithiated LNO to the oxidation of oxygen in hopes of verifying the mechanism of its degradation above 4.4 V and recently-reported signatures of O_2 formation [2]. We find that (1) lithium staging is necessary to computationally reproduce the lattice constants of the H3 phase, and (2) layered NiO₂ is thermodynamically unstable versus the formation of molecular lattice O_2 , albeit with only a small driving force. The origin of this instability is the antiferromagnetic coupling between reduced nickels. We conclude by investigating the energetics of oxygen loss and reconstruction at the surfaces of LNO and NiO₂ and find that the migration of Ni into the Li layer becomes immediately favorable upon surface oxygen loss.

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 A.S. Menon, *et al.*, PRX Energy **2**, 013005 (2021) <u>doi:10.1103/PRXEnergy.2.013005</u>.









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An evaluation of the barriers faced by various stakeholders in the EV battery value chain: can the law and policy in the European Union facilitate the transition to a sustainable circular economy?

King Men Teoh Universitetet i Oslo

Transportation is one of the largest emitters of greenhouse gas emissions (GhG) worldwide, accounting for 17% of global emissions. According to the Paris Agreement, emissions need to reduce by 45% by 2030 and reach net zero by 2050. European Green Deal sets the overarching aim of making the European Union climate neutral in 2050. Hence, achieving the targeted emission reductions, and more broadly to transition towards a sustainable future, requires a fundamental transformation of the energy and automotive sectors and of our societies.

As part of the interdisciplinary EMPOWER Project¹ that aims to investigate the role of electric vehicle (EV) batteries to enable a sustainable net-zero transition, the focus of my research is to investigate the legal framework in mobility to achieve a sustainable circular economy and develop a coherent regulatory framework both in Norway and the EU. In this paper, I aim to explore more specifically what barriers various stakeholders are facing, and how the law can contribute to addressing those barriers.

This paper will first examine the barriers faced by various stakeholders including consumers, manufacturers, and recyclers in the battery value chain to achieve a sustainable circular economy. Those barriers may include economic, legal, psychological, and educational.

This paper will then analyse the existing EU regulatory framework and the proposed new Regulation for batteries that will soon replace the 2006 Batteries Directive.² The purpose is to examine whether and how the proposed Regulation³ can contribute to tackle those barriers, thus, improving and making an effective change for the environment of EV batteries throughout their whole life cycle.

The next part of this paper will discuss opportunities as well as gaps and drawbacks of the proposed Regulation and make policy recommendations to overcome and address further the barriers to a transition to a sustainable circular economy for EV batteries.

The paper will end with conclusions and reflections on the need for further research.

REFERENCES[1] Dr Eléonore Maitre-Ekern, eleonore.maitre-ekern@jus.uio.no

³ European Commission, Proposal for a Regulation of the European Parliament and of the Council concerning Batteries and Waste Batteries, Repealing Directive 2006/66/EC and Amending Regulation (EU) No.2019/1020, COM(2020)798 final











¹ EMPOWER: Sustainable Batteries in Mobility – Empowering a net-zero energy transition <u>https://www.mn.uio.no/its/english/research/projects/empower/</u>

² Council Directive 2006/66/EC of 6 September 2006 on batteries and accumulators and waste batteries and accumulators and repealing Directive 91/157/EEC, OJ L 266/12

Application of organic cathodes for rechargeable multivalent batteries

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Rechargeable multivalent (Mg, Ca, Al) batteries are highly perspective battery technology due to elemental abundance and high capacity of metal anodes. However, lack of suitable cathode hosts has limited their practical application. Conventional inorganic hosts suffer from difficult multivalent cation insertion, tendency towards irreversible reactions and solvent co-intercalation, resulting in only a handful of inorganic cathode hosts with low practical energy densities.

Organic cathodes due to their soft and adaptable structures offer an option to circumvent these limitations. Within our group, we applied different organic compounds from the class of anthraquinone compounds in Mg, Ca and Al metal anode batteries and observed good electrochemical reversibility.¹⁻³ Electrochemical mechanism was studied using *ex situ* and SEM-EDS, which revealed presence of cation-anion pairs in the discharge cathodes (Figure 1). Cation-anion pairs mean electrolyte utilization in the electrochemical mechanism and would severely decrease the achievable practical energy density of the cells and should be addressed in the future research. Another pressing issue of multivalent cells is large overpotential of metal anodes limiting the performance and reproducibility of conventional half-cell tests. Use of symmetrical cells allows us to bypass this limitation and assess inherent performance of organics.⁴



Figure 1. Selected galvanostatic cycles for cycling of poly (anthraquinonyl sulfide) cathode with different metal anodes in half cell setup, Ca (blue), Mg (purple), Al (green) and Li (dashed black). On the right identified cations in the discharged cathodes by SEM-EDS.

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Operando ultrasonic signal evaluation for a lithium-ion battery

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The increasing need for green transportation has promoted the gradual dominance of lithium-ion batteries(LIBs) in the market due to their high energy density, low self-discharge, and long cycling life [1]. However, given the limited number of measured quantities, the effect of measurement noise, and the complicated aging mechanisms, the current battery management systems (BMS) may not be capable or sufficient enough to handle the public anxieties regarding fast charging [2] and electric vehicle range [3] etc. A push to develop new monitoring techniques for LIBs has led to spectacular advances across novel sensing techniques, with which the battery will no longer be simply a black box [4]. The ultrasonic sensors, which are widely used to detect defects (such as corrosion or cracks) that may not be visible from the outside, are employed to evaluate the internal states of a commercial pouch NCM battery. The employed pitch-catch inspection configuration is depicted in Figure 1. The whole system includes several functional units, such as the pulser/receiver, transducers, and display devices. The battery was placed inside a 25°C thermal chamber and operated with a constant current constant voltage (CCCV) charging and CC discharging. Simultaneously, the ultrasonic pulses, which was a rectangular pulse with 200V and a length of 250ns, was continuously sent from the pulser. The experimental results reveal that ultrasonic features, such as maximum amplitude and time-of-flight, undergo significant changes during battery operation. These features hold promise for determining battery states, and we aim to leverage them to develop effective and physics-guided BMS to ensure the safe and reliable operation of LIBs.



Figure 1. Schematic illustrations of ultrasonic testing with a pouch battery. Top: the experimental setups, including the signal generation and acquisition system and a pouch cell with transmitting and receiving piezos attached. Bottom left: the sound (represented by arrows) going through different layers of the cell, with some reflected and some transmitted. Bottom right: piezos of slice shape.

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Ethylene carbonate reaction pathways and their respective contributions to the solid electrolyte interphase in Li-ion batteries

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The solid electrolyte interphase (SEI) is vital to a high performing Li-ion battery. The composition of the SEI is an assortment of decomposition products, mainly from reduced additives or electrolyte species, such as ethylene carbonate (EC). During the operation of a Li-ion battery, the composition of the SEI evolves and continues to form, making it challenging to gain a complete understanding through post-mortem analysis alone. Analytical techniques monitoring the battery during operation, are needed to deconvolute the EC reaction pathways and their respective contributions to the SEI. Online Electrochemical Mass Spectrometry (OEMS) can sample the gas composition of a battery.¹ By sampling the volatile species from a battery cell during operation, an overview of voltage-dependent gas evolution processes is gained.

In this presentation, our focus is on two EC reaction pathways that occur on a model carbon electrode.² The first pathway, "EC ring-opening" pathway is initiated by hydroxides/alkoxides at potentials >1.5 V vs. Li⁺/Li.^{3,4} CO₂ evolution is linked to EC ring-opening and is here used as an identifier for the reaction. The second pathway, "EC reduction" pathway occurs <0.9 V vs. Li⁺/Li, where the reaction is identified via C₂H₄ evolution.⁵ Both reaction pathways contribute to the SEI. Additionally, the EC reaction pathways exhibit a competitive relationship, where EC ring-opening dominance results in suppression of the EC reduction pathway. The competing relationship of the two different EC reaction pathways is shown in Figure 1, where addition of EC ring-opening initiators (H₂O) increases CO₂, and decreases C₂H₄. The importance of considering every possible EC reaction pathway, not only the desired one, for SEI formation is highlighted together with a discussion of possible implications EC ring-opening has on a Li-ion cell.



Figure 1. Comparison between the total CO₂ and C₂H₄ evolution during the initial cyclic voltammetry cathodic sweep in a Glassy carbon | 1 M LiPF₆ EC:DEC | LiFePO₄ cell.

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New, faster, better, and beyond

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In this contribution, I will highlight three recent innovations from the platform for accelerated electrochemical energy storage research (PLACES/R) pertaining to all TRL. This presentation will highlight how to synthesize and upscale a new cell chemistry for Na-ion batteries in less than a month, and how to provide ample data for parametrization of full cells (TRL 1-3). I will demonstrate how we can accelerate the most time and cost intensive cell manufacturing process: formation of the SEI, through deploying AI control. This innovative formation process cuts the time for formation in half whilst delivering better performance across virtually all parameters at cells ranging from a few mAh to up to 100Ah. This novel process allows not just for fast and controlled formation but also allows for grading during formation (TRL 3-6). Finally, I will present an engineering framework for accelerating not just subsystems within a materials acceleration platform (MAP) but how to intelligently design MAPs. Through deployment of digital twins integrated into the fast intention agnostic learning server V2 (FINALES2) we can maximize operation efficiency of multiple integrated labs (TRL 6-9). This will be illustrated through accelerating battery testing by a factor of up to 100x.













Stress-driven propagation of lithium plating in commercial batteries

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The degradation of large-format lithium-ion batteries is highly sensitive to spatial distributions of temperature, pressure, material loading, and other variables. In our recent works, we have quantified accumulated dead lithium in separators and graphite electrodes harvested from automotive-grade batteries [1,2] using ⁷Li nuclear magnetic resonance spectroscopy. From these findings, we have proposed a revised, stress-driven mechanism that enables widespread lithium plating, even at modest state-of-charge of the full cell.

The prismatic cells studied in this work contain twin, wound jellyrolls. The curved and flat sections of the jellyrolls experience uneven stresses due to electrode (de)lithiation during cycling. The porous networks in the separators and negative electrodes, critical for ionic transport, are susceptible to crushing and deformation, particularly under high applied pressure [3]. Localized lithium plating is then possible and observed (as in Figure 1) where the ionic transport is hindered. This can be attributed either to severe potential swings in the affected regions or, in some cases, the overutilization of adjacent regions [4,5]. As lithium is plated and the deposits grow with continued cycling, increasing thickness corresponds to greater compression and stress, and lithium plating propagates laterally across the electrode.

This suggested mechanism is supported by spatially resolved, post mortem measurements of lithium plating, electrochemical state, and performance. A physics-based model is developed in COMSOL Multiphysics[®] to estimate the electrode potentials as dependent on a local defect. Plating potentials (<0 V vs. Li/Li⁺) are achieved at points along the surface of the negative electrode during cycling even when the overall SOC remains <65 %. Our studies suggest that external compression is critical to cycle life, even in prismatic cells with rigid casings. Pressure management is therefore an important concept for future cell and module designs, and local stress must be considered as a key risk factor for lithium plating.



Figure 1. Photographs of a compressed cell, jellyrolls, and harvested components. Schematics of intact (green) and degraded (red) separator and negative electrode regions.

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Using a reference electrode inside Li-ion cell to study the impact of the protocol on aging mechanisms

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Due to the massive deployment of lithium-ion batteries (LIBs) in EVs, special attention must be paid to safety and thus to understanding the aging mechanisms inside the cells. To meet this major challenge, the implementation of embedded sensors inside the batteries seems to be a key ally. As an electrochemical sensor, the reference electrode [1] provides interesting results in terms of degradation detection since it allows the potential of each electrode to be monitored individually. The objective of our study was to assess the impact of the aging protocol on the cell behavior, specifically on the lithium plating onset.

During the checkup, a slow discharge is performed, followed by a constant voltage at the lower battery voltage, in order to fully discharge the cell. During the CV step, the negative electrode is fully delithiated and its potential increases. Our study, involving a positive electrode of NMC 622 and Gr + 10% SiOx as the negative electrode, showed that the depth of discharge has an impact on the subsequent charge at a faster C-Rate. Our results showed that the behavior of the negative electrode in terms of potential is different whether the cell is fully discharged or not. After the checkup, the negative electrode fell below OV vs Li+/Li faster and for a longer period of time, which was favorable to the formation of lithium plating. With the reference electrode, we were able to analyze the impact of the protocol on the negative electrode potential in different aging conditions to monitor lithium plating formation.

This work was funded by the FOCUS Battery project of the CEA.



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Deciphering Li deposition and SEI with cryo-EM and cryo-ET

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Understanding in detail the behaviour of Li deposition and SEI formation is crucial for the rational design of stable Li metal anodes, but has remained tremendously challenging due to the extremely high sensitivity of metallic Li. [1] To address this issue, cryogenic electron microscopy (cryo-EM) has in recent years emerged as a powerful tool for visualizing sensitive Li deposition and SEI on the nanoscale. In our study, to understand the morphological evolution of Li nucleation and deposition under various current densities, we performed multiscale morphological characterization of Li deposits and the SEI using cryogenic transmission electron microscopy (cryo-TEM) combined with focused ion beam scanning electron microscopy (FIB/SEM). The Li deposits are found to be ball-shaped where the local charge density is low, while Li-whiskers appear where a high flux of Li-ions and electrons exists. Meanwhile, the Li-balls are concluded to be the origin of the Li-whiskers, and the ball-shaped deposits appear to be mostly amorphous while the Li-whiskers being highly crystalline. Moreover, the nanostructures and compositions of the SEI layer on Li balls and whiskers are different, with thin and LiFdominated SEI on Li-balls and thick and organic-enriched one on Li-whiskers. (Figure 1a) The distinction in SEI is further correlated to the Li nucleation and growth behaviors of these two types of Li deposits. [2] Moreover, to decipher the Li deposition and SEI evolution processes under an operando polymerized SEI which resulted in an ultra-high Coulombic efficiency of 99.97% for Li plating/stripping, we used cryo-TEM and cryogenic electron tomography (cryo-ET), complemented with operando electrochemical atomic force microscopy (EC-AFM), which demonstrated the morphological evolution of Li deposits from large-sized and low-tortuosity spheres to columns, together with thinning of the *operando* polymerized SEI layer from ~100 nm to 7 nm and self-healing capability. leading to efficient Listripping (i.e., with minimum "dead" Li) and non-continuous SEI formation. (Figure 1b) [3] These results provide new mechanistic understandings of Li deposition and SEI growth, which could guide the rational design Li metal anodes and interfaces toward stable operation.



Figure 1. Morphologies of Li deposits and SEI obtained with cryo-EM and cryo-ET.

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Complete and Selective recovery of lithium from EV lithium-ion batteries using oxalic acid as a leaching agent

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The development of electric vehicle is lead to a surge in battery demand, it doubled in 2021. The lithium nickel manganese cobalt oxide (NMC) cathode material remains the dominant technology of battery in the market [1]. This growth of e-mobility has caused a significant increase in the battery key metals demand such as nickel, cobalt, copper, and lithium. Concern about raw material supply is growing, and lithium was included among the critical raw materials in 2020 by the European Union [2]. The new regulation around batteries is requesting a better end-of-life management, considering recycling as a mandatory operation. A recovery target of lithium is set at 70% by 2030. Besides, recycled lithium should be implemented in new batteries produced in Europe at a minimum level of 6% by 2030. Moreover, the price rose from 7000 \$/t of lithium carbonate to 26000 \$/t in November 2022. Current hydrometallurgical methods do not achieve very high recovery of the element, recovered at last in the process, and some losses are occurring at each step. New recycling strategies are trying to lift the importance of lithium by recovering selectively the element in the first step before any other valuables metals.

In this work, the black mass composed of the anode and cathode active material (Figure 1a) is processed using oxalic acid as a leaching agent. The oxalic acid acts as a leaching agent and reducing agent, dissolving the metal oxides in the solution. Then, the oxalate ions react with the metal ions forming strong chelate complexes. 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. Nickel, cobalt, and manganese oxalates are insoluble and remained in the solid residue, while lithium oxalate was dissolved in the solution. Using a design of experiments to optimize the operation, optimal parameters were identified as 60°C, 60 min, 0.6 M oxalic acid with a solid-to-liquid ratio of 50 g/L. This led to a very successful selective separation with a leaching yield for lithium of 98.8%, while less than 0.5 % of cobalt and nickel, and 1.5% of manganese were leached. The leaching residue was analyzed with XRD and the presence of metal oxalate was confirmed (Figure 1b). Moreover, aluminum was completely dissolved, which is a phenomenon not reported previously. It would constitute an advantage to the subsequent recycling operations.



Figure 1. XRD pattern of the black mass a) and the leaching residue b).

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Poster Presentations









Nr.	Abstract title, authors and affilia
P1	Parameterisation of electrical and thermal models at module-level for a Li-ion battery digital twin simulation platform Olatz Lizaso-Eguileta ^{1,2,3} Josu Olmos ¹ , Iñigo Gandiaga ¹ , Eduardo Miguel ¹ , Unai Iraola ¹ , Igor Cantero ³ , ¹ Ikerlan Technology Research Centre, Basque Research and Technology Alliance (BRTA), Arrasate-Mondragon, Basque Country, Spain ² Mondragon Unibertsitatea, Faculty of Engineering, Arrasate-Mondragon, Basque Country, Spain ² Cegasa Energía, R&D Department, Vitoria, Basque Country, Spain
P2	State-of-safety (SoS) algorithm for Li-ion batteries based on internal novel sensing technologies <u>Josu Olmos¹</u> , Iñigo Gandiaga ¹ , Ainhoa Mugertza ¹ ¹ Ikerlan Technology Research Centre, Basque Research and Technology Alliance (BRTA), P ^o J.M. Arizmendiarrieta 2, 20500 Arrasate-Mondragon, Basque Country, Spain
Р3	Computational search for novel solid-state electrolytes <u>Zakaryan Hayk¹</u> , Dallakyan Olgert ¹ , Hunanyan Areg ¹ , Aghamalyan Misha ¹ ¹ Computational Materials Science Laboratory, Yerevan State University, Yerevan, Republic of Armenia
Ρ4	Novel sensing technology for li-ion batteries: auxiliary reference electrodes printed on cell separators <u>P. Di Prima¹</u> , D. Dessantis ¹ , S. Bellani ² , H. Beydaghi ² , M. Santarelli ¹ , F. Bonaccorso ² , S. Bodoardo ³ ¹ Politecnico di Torino, (Dept. Of Energy), 10129-Turin, Italy ¹ BeDimensional S.p.A., Genova, 16163, Italy ³ Politecnico di Torino, (Dept. Of Applied Science and Technology), 10129-Turin, Italy
Р5	Integration of Temperature and Pressure Sensing Functionalities into Li-ion Pouch Cell on an Industry-Relevant Scale <u>Bernd Eschelmüller¹</u> , Gregor Glanz ¹ , Katja Fröhlich ¹ ¹ Battery Technologies, AIT Austrian Institute of Technology GmbH, Vienna, Austria
Р6	Phase separated polymer electrolytes for Li-ion batteries using oligomeric carbonates <u>Samuel Emilsson¹</u> , Vidyanand Vijayakumar ² , Jonas Mindemark ² , Mats Johansson ¹ ¹ Department of Fibre and Polymer Technology, KTH Royal Institute of Technology, Stockholm, Sweden ² Department of Chemistry - Ångström Laboratory, Uppsala University, Uppsala, Sweden



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P7	Accelerating the discovery of organic battery materials: from atomistic modelling to artificial intelligence <u>C. Moyses Araujo^{1,2}</u> , Rodrigo P. de Carvalho ^{2,3} , Cleber F. N. Marchiori ¹ and Daniel Brandell ³ ¹ Department of Engineering and Physics, Karlstad University, 65188 Karlstad, Sweden.
	³ Department of Chemistry - Ångström Laboratory, Uppsala University, Box 538, 751 21 Uppsala, Sweden
P8	Fibre optical sensors for operando monitoring of internal processes in Li-ion and Na-ion batteries <u>Irem Tanyeli</u> ¹ , Fredrik Cognell ¹ , Saima Zaman ¹ , Radmila Batinic ¹ , Elin Langhammer ¹ ¹ Insplorion AB, Arvid Wallgrens backe 20, Göteborg, Sweden
Р9	INSTABAT - Smart multi-sensor plattform Franchi Romain¹ , Olivier Raccurt ² , Cedric Septet ³ , Sylvie Genies ⁴ ^{1,2,3,4} Univ. Grenoble Alpes, CEA LITEN, Electricity and Hydrogen for Transportation Division (DEHT), 1Laboratory of Power Electronics and Energy Management (L2EP) ^{2,3,4} Laboratory of Post-Mortem Analysis (LAP), F-38054 Grenoble, France
P10	Hybrid polymer-liquid lithium ion electrolytes: effect of porosity on the ionic and molecular mobility Martina Cattaruzza ¹ , Yuan Fang ² , István Furó ² , Göran Lindbergh ³ , Fang Liu ⁴ and Mats Johansson ¹ ¹ Division of Coating Technology, Department of Fibre and Polymer Technology, KTH Royal Institute of Technology, SE-100 44 Stockholm, Sweden ² Division of Applied Physical Chemistry, Department of Chemistry, KTH Royal Institute of Technology, SE-100 44 Stockholm, Sweden ³ Division of Applied Electrochemistry, Department of Chemical Engineering, KTH Royal Institute of Technology, SE-100 44 Stockholm, Sweden ⁴ Division of Materials and Manufacture, Department of Industrial and Materials Science, Chalmers University of Technology, SE-412 96 Gothenburg, Sweden7
P11	The GigaGreen Project. Towards the sustainable giga-factory: developing green cell manufacturing processes <u>Elisa Ravesio¹</u> , Giorgio Montinaro ¹ , Daniele Versaci ¹ , Federico Bella ¹ , Silvia Bodoardo ¹ ¹ Dip. Applied Science and Technology (DISAT), Politecnico di Torino, C.so Duca degli Abruzzi 24, 10029 Torino, Italy
P12	Raman spectroscopy of NMC and first principles study of LixNiO2 cathodes for Li-ion batteries Javier García-Alonso ¹ , Rita Magri ² , M.M. Mridha ² , S. Yousuf ² , Ruth Martinez-Casado ² , David Maestre ² , Bianchi Méndez ² ¹ UCM, Faculty of Physics, Department of Physics of Materials, Madrid, Spain ² UNIMORE, FIM Department University of Modena and Reggio Emilia, Modena, Italy
P13	Challenges and opportunities for copper hexacyanoferrate in rechargeable aqueous Zn-ion batteries <u>Mario Valvo¹</u> , Mikaela Görlin ¹ , Dickson O. Ojwang ¹ , Ming-Tao Lee ¹ , Viktor Renman1, Cheuk-Wai Tai ² ¹ Department of Chemistry – Ångström Laboratory, Uppsala University, SE-75121 Uppsala, Sweden ² Department of Materials and Environmental Chemistry, Stockholm University, SE-10691, Stockholm, Sweden
P14	Modelling self-healing binders for silicon anodes <u>R. Magri¹</u> , R. Maji ² , M. A. Salvador ¹ , A. Ruini ¹ , E. Degoli ² ¹ Dipartimento di Scienze Fisiche, Informatiche e Matematiche, Università di Modena e Reggio Emilia, Via Campi 213/A, 41125 Modena, Italy ² Dipartimento di Scienze e Metodi Dell'Ingegneria, Università di Modena e Reggio Emilia, Via Amendola 2, I-42122, Reggio Emilia, Italy







P15	Automated electrolyte formulation and coin cell assembly for high-throughput lithium-ion battery research Jackie T. Yik ¹ , Leiting Zhang ¹ , Jens Sjölund ² , Xu Hou ¹ , Per H. Svensson ^{3,4} , Kristina Edström ¹ , Erik J. Berg ¹ ¹ Department of Chemistry – Ångström Laboratory, Uppsala University, Uppsala, Sweden ² Department of Information Technology, Uppsala University, Uppsala, Sweden ³ Chemical and Pharmaceutical Development, RISE Research Institutes of Sweden, Södertälje, Sweden ⁴ Applied Physical Chemistry, Department of Chemistry, KTH Royal Institute of Technology, Stockholm, Sweden
P16	Self-healing ionic-liquid-based electrolytes <u>Zviadi Katcharava¹</u> , Chenming Li ¹ , Rajesh Bhandary ¹ , Anja Marinow ¹ , <u>Wolfgang H. Binder¹</u> ¹ Macromolecular Chemistry, Institute of Chemistry, Martin-Luther University Halle-Wittenberg, Von-Danckelmann-Platz 4, D-06120 Halle (Saale), Germany
P17	A discrete element analysis of the mechanical behaviour of an electrode active layer <u>Axel Lundkvist¹</u> , Per-Lennart Larsson ¹ , Erik Olsson ² ¹ Department of Engineering Mechanics, KTH Royal Institute of Technology, Stockholm, Sweden ² Department of Engineering Sciences and Mathematics, Division of Solid Mechanics, Luleå University of Technology, Luleå, Sweden
P18	My research activity with kalium <u>Sabrina Trano¹</u> , Lucia Fagiolari ¹ , Daniele Versaci ¹ , Julia Amici ¹ , Carlotta Francia ¹ , Federico Bella ¹ , Silvia Bodoardo ¹ ¹ Department of Applied Science and Technology, Politecnico di Torino, Corso Duca degli Abruzzi 24, 10129 – Torino, Italy
P19	Development of an ORP-EIS sensor for <i>in situ</i> SoX determination <u>Benny Wouters</u> , Raf Claessens ¹ , Xia Zeng ² , Pavlo Ivanchenco ² , Maitane Berecibar ² , Annick Hubin ¹ ¹ Vrije Universiteit Brussel, Research Group Electrochemical and Surface Engineering, Pleinlaan 2, 1050 Brussels, Belgium ² Vrije Universiteit Brussel, Electromobility Research Centre, Pleinlaan 2, 1050 Brussels, Belgium
P20	Fibre optical detection of lithium and sodium plating in intercalation batteries Fredrik Björefors ¹ , Jonas Hedman ¹ , Ronnie Mogensen ¹ , Reza Younesi ¹ ¹ Dept. of Chemistry – Ångström Laboratory, Uppsala University, Box 538, SE-751 21, Uppsala, Sweden. Email: <u>fredrik.bjorefors@kemi.uu.se</u>
P21	A holistic approach on the feasibility of garnet-based all solid-state lithium batteries Ignacio Cuevas ¹ , Funeka Nkosi ¹ , Kristina Edström ¹ , Mario Valvo ¹ ¹ Department of Chemistry – Ångström Laboratory, Uppsala University, SE-75121 Uppsala, Sweden
P22	In-Situ liquid-state NMR investigations of lithium-ion battery electrolyte decomposition <u>Wandi Wahyudi</u> ¹ , Jonas Mindemark ¹ , Kristina Edström ¹ ¹ Department of Chemistry – Ångström Laboratory, Uppsala University, SE-75121 Uppsala, Sweden







P23	OCV hysteresis in NIMH - a structural investigation Jenny Börjesson Axén ¹² , Gustav Ek ³ , Alice Gratrex ¹ , Göran Lindbergh ¹ , Dag Noréus ⁴ , Ingmar Persson ⁵ , Helen Y. Playford ⁶ , Kajsa G. V. Sigfridsson Clauss ⁷ , Jakob Thyr ⁸ , Erika Widenkvist Zetterström ⁹ ¹ Department of Chemical Engineering, Division of Applied Electrochemistry, School of Chemistry Biotechnology and Health, KTH Royal Institute of Technology, SE-100 44 Stockholm, Sweden ² Nilar AB – Bönavägen 55, SE-806 47 Gävle, Sweden ³ Department of Chemistry - Ångström Laboratory, Uppsala University, Box 523, Uppsala SE-751 20, Sweden ⁴ Department of Materials and Environmental Chemistry, Stockholm University, Svante Arrhenius Väg 16 C, SE-114 18 Stockholm, Sweden ⁵ Department of Molecular Sciences, Swedish University of Agricultural Sciences, P.O. Box 7015, SE-750 07 Uppsala, Sweden ⁶ ISIS Neutron and Muon Source, Rutherford Appleton Laboratory, Harwell Campus, Didcot, OX11 0QX, UK 7 MAX IV Laboratory, Lund University, P.O. Box 118, SE-221 00 Lund, Sweden ⁷ Department of Materials Science and Engineering, Solid State Physics, Ångström Laboratory, Uppsala University, Box 35, SE-751 03, Uppsala, Sweden ⁸ Graphmatech AB – Mältargatan 17, SE-753 18 Uppsala, Sweden
P24	Self-healing polymer integration into Core/Shell NMC cathode material <u>E. Guney</u> ¹ , <u>S. Krüger</u> ² , N. Saini ² , N. Yuca ¹ , B. Saruhan ² ¹ ENWAIR Energy Technologies Corporation, Maslak, 34469 Istanbul, Turkey ² Institute of Materials Research, German Aerospace Center (DLR), Linder Hoehe 51147, Cologne, Germany
P25	Enhanced performance of li-ion battery electrodes protected by atomic layer deposited ultrathin films <u>K. Frohlich^{1,2}</u> , P. P. Sahoo ¹ , A. Güneren ^{1,3} , B. Hudec ² , M. Mikolášek ⁴ , A. Nada ¹ , M. Precnerová ¹ , M. Mičušík ⁵ ¹ Centre for Advanced Materials Application, Slovak Academy of Sciences, Bratislava, Slovakia ¹ Institute of Electrical Engineering, Slovak Academy of Sciences, Bratislava, Slovakia ³ Institute of Inorganic Chemistry, Slovak Academy of Sciences, Bratislava, Slovakia ⁴ Institute of Electronics and Photonics, Slovak University of Technology, Bratislava, Slovakia ⁵ Polymer Institute, Slovak Academy of Sciences, Bratislava, Slovakia
P26	Non-flammable localized highly concentrated electrolyte for lithium-ion batteries <u>Wessel van Ekeren</u> ¹ , Marcelo Albuquerque ¹ , Gustav Ek, Ronnie Mogensen, William R. Brant, Luciano T. Costa, Daniel Brandell and Reza Younesi ¹ Department of chemistry-Ångström Laboratory, Uppsala University, Box 538, Uppsala SE-751, Sweden ² Physical Chemistry Department, Institute of Chemistry, Fluminense Federal University, Campus Valonguinho, Brazil
P27	Hard carbon from softwood kraft lignin for sodium-ion batteries <u>Omid Hosseinaei¹</u> , Habtom Desta Asfaw ² , Stacy Trey ¹ , Maciej Wysocki ¹ ¹ RISE Research Institutes of Sweden, Drottning Kristinas väg 61, 114 28 Stockholm, Sweden ² Department of Chemistry - Ångström Laboratory, Uppsala University, Box 538, 751 21 Uppsala, Sweden
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P30	Heating element on the pouch cell <u>Doniyor Urishov</u> ^{1,*} , Johannes Ehrlich ² , Simon Müller, ³ Tuomas Happonen ¹ , Mari Ylikunnari ¹ , Marja Vilkman ¹ ¹ VTT Technical Research Centre of Finland Ltd P.O. Box 1000, FI-02044 VTT, Finland ² Fraunhofer Institute for Silicate Research ISC, 97082 Würzburg, Germany ³ Bern University of Applied Sciences, 3400 Burgdorf, Switzerland
P31	Improved electrochemical performance enabled by solution-based synthesis: cathodes, anodes, and electrolytes <u>Dries De Sloovere</u> ¹ , Andreas Paulus ¹ , Satish Kumar Mylavarapu ¹ , Bjorn Joos ¹ , An-Sofie Kelchtermans ¹ , Jonas Mercken ¹ , Marlies K. Van Bael ¹ , An Hardy ¹ ¹ UHasselt, Institute for Materials Research (IMO-Imomec) and Imec division Imomec, DESINe, Agoralaan, building D, 3590 Diepenbeek, Belgium. EnergyVille, Thor Park 8320, 3600 Genk, Belgium
P32	Operando nuclear magnetic resonance study of the lithium plating mechanism for the optimization of Li-ion battery fas <u>Abdelmounaim Akchach¹</u> , Sylvie Genies ¹ , Marion Chandesris ¹ , Michel Bardet ² ¹ Univ. Grenoble Alpes, CEA, Liten, Department of Electricity and Hydrogen for Transport, F-38000 Grenoble, ² Univ. Grenoble Alpes, CEA, IRIG, Department of Physics, F-38000 Grenoble, France
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P37	Enhancing the performance of Na2FeP2O7 and Na0.67MnO2 cathodes for sodium-Ion batteries <u>Gints Kucinskis</u> , Inara Nesterova, Beate Kruze, Gunars Bajars Institute of Solid State Physics, University of Latvia
P38	Polyanion Insertion Material as a Catalyst for Oxygen Electrocatalysis <u>Ritambhara Gond</u> , Mikaela Görlin, Jiefang Zhu Department of Chemistry - Ångström Laboratory, Uppsala University, Box 538, 751 21 Uppsala, Sweden



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**Department of Electrical Engineering, Chalmess 7, Engineering, 34286 Gothenburg, Sweden **Department of Electrical Engineering, Chalmess 7, 2010 Muressity of Erechnology, 41296 Gothenburg, Sweden P40 SMART BMS Testing for advanced SoX estimation Mikel Oyarbidg, Joanes Lorente ¹ , Johannes Ziegler ¹ , Pavlo Vanchenko ² **OEDETC Energy Storage, FM Miramón, 196. 20014 Donostia San Sebastián, Spain **raunhofer Institute for Silicate Research ISC, Würzburg, Germany **rije Universiteit Furssel, Pleinian 21050 Brussels, Belgium P41 Synthesis of Glass-ceramic Li2S-P2S5 based electrolyte for solid-state batteries Leo Sjörén ¹ , Ignacio Cuevas ¹ , Funeka Mkosi ¹ *Department of Chemistry – Angström Laboratory, Uppsala University, SE-75121, Uppsala, Sweden P42 2.4 V Amphoteric rechargeable Zn-MnO2 battery Anzelma Zukus ¹ , Ramona Durea ³ , Martins Vanags ¹ *The Institute of Materials and Surface Engineering, Riga Technical University, Latvia P43 Integrable multi sensor array for improved aging detection in lithium-ion battery cells Simon Feller ¹ , Johannes Ziegler ¹ , Johannes Ehrlich ¹ , Philip Daubinger ⁴ , Beatrice Laurenh ¹ , Andre Bagheri ¹ , Silvia Bodoardo, ² and Francesco Bonaccorso P444 Integration of printed graphene-based reference electrodes in lithium-ion batteries for advance Hosein Beydath ¹ , Sebastian Dellani, ¹ Plera Dirima, ¹ Davide Dessantis, ⁴ Beatrice La	
+Department of Electromobility, Volvo Group Trucks Technology, 40308 Gothenburg, Sweden P40 SMART BMS Testing for advanced SoX estimation Mikel Oyarhide, Joanes Lorente ¹ , Johannes Ziegler ¹ , Pavlo Ivanchenko ¹ *CUETEC Energy storage, P7 Miramón, 196. 20014 Donostia San Sebastián, Spain *Cuence Research ISC, Wurzburg, Germany *Vrije Universiteti Brussel, Pleinlaan 21050 Brussels, Belgium P41 Synthesis of Glass-ceramic Li2S-P2S5 based electrolyte for solid-state batteries Leo Sjören ¹ , Ignacio Cuevas ¹ , Funka Nkos ¹¹ *Department of Chemistry – Angström Laboratory, Uppsala University, SE-75121, Uppsala, Sweden P42 2.4 V Amphoteric rechargeable Zn-MnO2 battery Anzelms Zukus ¹ , Ramona Durea ¹ , Martins Vanags ¹ *The Institute of Materials and Surface Engineering, Riga Technical University, Latvia P43 Integrable multi sensor array for improved aging detection in lithium-ion battery cells Simon Feiler ¹ , Johannes Englich ¹ , Neumerplat 2, 97082 Wuerzburg ¹ CEA Grenoble, 17 Av. des Martyrs, 38000 Grenoble, France P44 Integration of printed graphene-based reference electrodes in lithium-ion batteries for advance Hossein Beydaphi ¹ , Sebastiano Bellani ¹ , Piera Di Prima, ¹ Davide Dessantis, ⁴ Beatrice Laurenti, ¹ Ahmad Bagheri, ¹ Slivia Bodoardo, ² and Francesco Bonaccorso I JBeDimensional S.p.A., Via Lungotorrente secca 30, 6163 Genova, Italy *Department of Applied Science and Technology (DISAT). Politecinci di Torino, C. so Duca degli Abruzzi 24, 10129, Torino, Italy P45 Effective scientific data sharing within BATTERY 2030+ Fracols Lidr ¹ , Valeria Granata ¹ , Xing Wang ² , Giova	
P40 SMART BMS Testing for advanced SoX estimation Mikel Ovarbide, Joanes Lorente ¹ , Johannes Ziegler ³ , Pavlo Ivanchenko ¹ ¹ CIDETEC Energy storage, P7 Miramón, 196 - 20014 Donostia San Sebastián, Spain ¹ Fraunhofer Institute for Silacte Research ISC, Wurzburg, Germany ¹ Vie Universiteit Brussel, Pleinlaan 21050 Brussels, Belgium P41 Synthesis of Glass-ceramic Li2S-P2S5 based electrolyte for solid-state batteries Leo Silfrén ¹ , Ignacio Cuevas ¹ , Funka Nkos ¹¹ ¹ Department of Chemistry – Ångström Laboratory, Uppsala University, SE-75121, Uppsala, Sweden P42 2.4 V Amphoteric rechargeable Zn-MNO2 battery Arzelms Zukus ¹ , Ramona Durea ¹ , Martins Vanags ¹ ¹ The Institute of Materials and Surface Engineering, Riga Technical University, Latvia P43 Integrable multi sensor array for improved aging detection in lithium-ion battery cells Simon Feiler ¹ , Johannes Ziegler ¹ , Johannes Ehrlich ¹ , Philip Daubinger ¹ , Bernhard Brunner ¹ , Holger Böse ¹ , Antoine Latour ² , Gerhard Domann ¹ ¹ Traunhofer Institute for Silica Research (ISC), Neumerplat 2, 97082 Wuerzburg ² CEA Grenoble, 17 Av. des Martyrs, 38000 Grenoble, France P44 Integration of printed graphene-based reference electrodes in lithium-ion batteries for advance Hossein Beydaghl ¹ , Sebastiano Bellani, ¹ Piera Di Prima, ² Davide Dessantis, ³ Beatrice Laurenti, ¹ Ahmad Bagheri, ¹ Silvia Bodoardo, ² and Francesco Bonaccorso 1BeDimensional S, D, A, Via Lungot	
Mikel Oyarbide, Joanes Jorente ¹ , Johannes Ziegler ³ , Pavlo Ivanchenko ³ ¹² CDETEC Energy storage, PP Miramón, 196. 20014 Donostia-San Sebastián, Spain ¹² Fraunhofer Institute for Silicate Research ISC, Wurzburg, Germany ¹⁴ Vrije Universiteit Brussel, Pleinlaan 21050 Brussels, Belgium P41 Synthesis of Glass-ceramic Li2S-P2S5 based electrolyte for solid-state batteries Leo Sibrén ¹ , Ignacio Cuevas ¹ , Funeka Nkosi ¹ ¹⁵ Department of Chemistry – Ångström Laboratory, Uppsala University, SE-75121, Uppsala, Sweden P42 2.4 V Amphoteric rechargeable Zn-MnO2 battery Anzelms Zukus ¹ , Ramona Durea ¹ , Martins Vanags ¹ ¹⁵ The Institute for Materials and Surface Engineering, Riga Technical University, Latvia P43 Integrable multi sensor array for improved aging detection in lithium-ion battery cells Sinnor Feller ¹ , Johannes Enrich ¹ , Philip Daubinger ¹ , Bernhard Brunner ¹ , Holger Böse ¹ , Antoine Latour ² , Gerhard Domann ¹ ¹⁴ Fraunhofer Institute for Silicate Research (ISC), Neunerplatz 2, 97082 Wuerzburg ¹⁴ CEA Grenoble, 17 Av. des Martyrs, 38000 Grenoble, France P44 Integration of printed graphene-based reference electrodes in lithium-ion batteries for advance Hossein Beydaghl, ¹ Sebastiano Bellan ¹ , Piera Di Prima ³ , Davide Dessantis, ² Beatrice Laurent ¹ , Ahmad Bagheri, ¹ Silvia Bodoardo, ³ and Francesco Bonaccorso BebDimensiond Sp.Av, Via Lungotorrent sesca 30, 16163 G	
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	¹ Flanders Make
	² Flanders Make
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	¹ Flanders Make
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	Mian Mohammad Arsalan Asif ¹ , Federico Bribiesca Argomedo ¹ , Vincent Heiries ²
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	² CEA Grenoble, Grenoble, France
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	Daniel Sethio ¹ , Jolla Kullgren ¹ , Kersti Hermansson ¹
	1 Department of Chemistry – Ångström, Uppsala University
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	Guiomar Hernández ¹ , Tamara Patranika ¹ , Kristina Edström ¹
	1 Department of Chemistry – Ångström Laboratory, Uppsala University 751 21 Uppsala, Sweden
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	Emina Hadzialic ¹ , Helmut Kühnelt ¹ , Francesco-Saverio Mastropierro ¹ , Alexander Ryzhov ¹
	¹ AIT Austrian Institute of Technology GmbH, Center for Low-Emission Transport, Vienna, Austria
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	Peter N. O. Gillespie ¹ . Deborah Prezzi ¹ . Elisa Molinari ²
	1 CNR-NANO S3, Modena, Italy
	2 Università degli studi di Modena e Reggio Emilia, Modena, Italy
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	Cédric Loubat ¹ S Malburet E Briée A Graillot
	¹ SPECIFIC POLYMERS, Castries, France – www.specificpolymers.com
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ergy density of Li-Metal batteries





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	¹ ID31 beamline, ESRF, 71 Av. des Martyrs, 38000 Grenoble, France ² Finden Limited, Merchant House, 5 East St Helens Street, Abingdon, OX14 5EG, United Kingdom
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	¹ Donan M. Carisson ⁻ , Hamid Hajiyani ⁻ , Nenzat Safael ⁻ and Felix Hanke ⁻ 1Dassault Systèmes Deutschland GmbH, Am Kabellager 11-13, 51063 Köln, Germany ² Dassault Systèmes UK Ltd, Cambridge Science Park, Cambridge CB4 OWN, UK
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	1 Karlsruhe Institute of Technology (KIT), Straße am Forum 7, 76131 Karlsruhe, Germany 2 Helmholtz Institute Ulm, Electrochemical energy storage (HIU), Helmholtzstraße 11, 89081 Ulm, Germany
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	¹ Department of Chemical Engineering, Boğaziçi University, Bebek, Istanbul, Türkiye ² R&D and Engineering, Siro Energy, Gebze, Kocaeli, Türkiye
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	² Sustainable Chemistry Unit, University of Oulu, 90570 Oulu, Finland



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	Daniele Costa ¹ , Maeva Lavigne Philippot ¹ , Maitane Berecibar ¹ and Maarten Messagie ¹
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PARAMETERISATION OF ELECTRICAL AND THERMAL MODELS AT MODULE-LEVEL FOR A LI-ION BATTERY DIGITAL TWIN SIMULATION PLATFORM

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Deployed Li-Ion Batteries (LIBs) are becoming increasingly large in scale and can consist of hundreds or thousands of individual cells. That means that many cells are connected to obtain these great energy values [1]. When these LIBs are in operation, there are some cell-to-cell unbalances concerning the temperature or State of Charge (SoC) of the cells composing every module. Those affect the performance of the LIBs and even their degradation. Currently, the module-level performance is evaluated based on single cell models, or averaged operating conditions, thus hindering the appropriate analysis of cell-to-cell variations. This work proposes module-level integrated electrical and thermal models based on equivalent circuits. A methodology for parameterising these models is presented, and an experimental validation platform is presented.

The execution of accurate heavy models with high-level of complexity requires computational capacity, which goes beyond the capabilities of conventional BMS solutions, thus leading to an implicit trade-off between accuracy and computation requirements. In this context, tools such as Digital Twin (DT) [2], together with Cloud and Internet of Things based technologies, are used to extend this computational capacity in favour of advanced modelling capabilities. This DT environment enables the implementation of central communication and network technologies, such as virtualisation and real-time monitoring, and, consequently, detects anomalies in the operation of the deployed cells by storing all the data in a single database.

Starting from the well-known cell-level models developed and already validated, the proposed approach to extrapolate these models to the module-level has been further detailed. In this way, the proposed models based on equivalent circuits are integrated into a Cloud-based Digital Twin Simulation Platform (DTSP). A methodology to parameterise each model of the DTSP is presented where the electrical model is parameterised at the cell-level and run as a co-simulation of every individual cell and the thermal model is tailored at the module-level.

To parametrise the heat transfer, a Computational Fluid Dynamics (CFD) based model has been designed. This model allows to obtain in sufficient detail the parameters linked to the heat transfer by natural convection and radiation. These parameters are then used in the tunning of a lumped parameter module-level Thermal Model, which ultimately represent a sort of reduced order model able to be deployed on a cloud environment.

With the contribution of this paper, it will be verified if the detailed simulation of each cell leads to more accurate estimations and information on the state of the entire module, even at points where there is no sensor measurement.



Figure 1. Schematic diagram of the proposed DTSP validation platform.

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STATE-OF-SAFETY (SoS) ALGORITHM FOR LI-ION BATTERIES BASED ON INTERNAL NOVEL SENSING TECHNOLOGIES

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The broader adoption of Li-ion Batteries (LiB) in a wide range of applications (including stationary and mobility ones) is a necessary step ahead to comply with the objectives of the green transition. However, simultaneously, the spread of these systems is increasing the safety requirements, as avoiding devastating events such as thermal runaway becomes essential [1]. In this regard, some countries are already tightening the legislations to increase user protection against catastrophic events of LiBs. For instance, China set in January 2021 a new standard for electric vehicles (GB/T 38031), which imposes a minimum time of 5 minutes between a thermal runaway warning is provided to the passengers, and the batteries start getting fire [2].

In this context, it is clear that a comprehensive monitoring of the battery state to prevent non-safe and devastating events is necessary to increase the reliability on LiBs. The approach proposed in this study aims at increasing the real time monitoring of LiBs, e.g., by measuring the temperature, pressure, and impedance of the cells (which are not typically monitored by commercial Battery Management Systems).

This increased knowledge of the real time system variables may help in developing more advanced and reliable LiB state algorithms. In this regard, this paper proposes a State-of-Safety (SoS) algorithm. The SoS is claimed to be a modular concept that represents the actual safety state of the LiB. The proposed state algorithm is defined between 0 and 1, being 0 a critically LiB unsafe state and 1 a state guaranteeing safety. In order to quantify the safety state, the SoS is divided into several subfunctions, each of them linked to a potential and measurable risk. Among others, these risks include voltage, temperature, current, pressure and impedance related safety issues. Critical safety limits are defined for each measurable risk, what allows quantifying the safety state of each corresponding SoS component. Eventually, the overall LiB SoS is derived by gathering together the individual states. Figure 1 shows the overall scheme of the proposed SoS algorithm.

Further information regarding the safety limits of each monitored variable, and a practical example of the SoS implementation will be given in the final version of the paper. The practical implementation will also show the added value of monitoring novel variables of the battery (e.g., acoustics, pressure, and impedance).



Figure 1. General scheme of proposed State of Safety (SoS).

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COMPUTATIONAL SEARCH FOR NOVEL SOLID STATE ELECTROLYTES

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In today's rapidly advancing technological landscape, energy storage systems that offer high energy density and fast charging capabilities are essential for modern devices and machines. While present Li-ion batteries with liquid electrolytes have reached their developmental limits, all-solid-state batteries are widely regarded as the future of energy storage systems. However, the currently known solid-state electrolytes such as sulfides, oxides, borates, etc., do not satisfy all the performance requirements, including high ion conductivity and compatibility with anode materials, needed for broad implementation in various applications [1]. Among the promising solid-state electrolytes are halides with monoclinic crystal systems. Stable Li3MH6 structures have already been experimentally or theoretically discovered in several halide systems such as Li-M-H (where M=Yb, Al, Sc, La, and H=F, Cl, Br, I) [2]. In this study, we leverage our chemical intuition, along with a data-mined substitution prediction methodology [3], to explore potential structures that could be thermodynamically stable in the Li-M-H (M=In, Ga, La, and H=F, Cl, Br, I) systems. Our analysis uncovered 19 structures with Li3MH6, and their stability was calculated using Density Functional Theory. Notably, five novel stable materials emerged, namely Li3InI6, Li3GaBr6, Li3Gal6, Li3LaF6, and Li3LaCl6. We evaluated the ionic conductivity and activation energy using ab-initio molecular dynamics, combined with machine learning interatomic potentials (MLIP) [4]. Our results showed that these novel materials exhibit high ion conductivity and low activation energy, making them a promising candidate for solid-state electrolytes.

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INSTABAT sensibat



NOVEL SENSING TECHNOLOGY FOR LI-ION BATTERIES: AUXILIARY REFERENCE ELECTRODES PRINTED ON CELL SEPARATORS

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Despite the increasing interest of automotive industry in electrical vehicles, battery lifetime falls below consumer expectation for long-term applications. Degradation of Li-ion cells can be caused by both chemical and mechanical factors, leading to capacity loss and impedance increase causing the failure of the cells at delivering and storing electrical energy at satisfactory rate [1]. In this contest, the H2020 Project SENSIBAT [2] aims to develop a sensing technology for Li-ion batteries that measures in real-time the internal battery cell parameters, such as temperature, pressure, anode and cathode potentials, as well as the impedances of cell elements and related interfaces through Electrochemical Impedance Spectroscopy (EIS). The data and insights from these new sensing technologies will be used for the development of advanced state estimator functions based on an improved understanding of how, where and when degradation and failure mechanisms occur.

In order to study the anode and cathode behavior in working conditions, an internal reference electrode can provide fundamental information; therefore, a novel sensing technology consisting of an auxiliary reference electrode printed directly atop the separators, has been developed within SENSIBAT project. A sensor working as reference electrode must possess stable equilibrium potential in the cell working conditions: for this reason, two different active material chemistries (Lithium Iron Phosphate -LFP- and Lithium Titanate Oxide -LTO-), showing two-phase reaction behavior, have been selected to formulate out printed sensors [3]. Different materials, including single-/few-layer graphene (SLG/FLG), reduced graphene oxide (RGO), carbon black (CB), were evaluated as electrically conductive materials, while assessing the printability of the resulting electrode compositions. The structural and morphological properties of the produced electrodes were characterized with X-Ray Diffraction (XRD), Scanning Electron Microscope (SEM) and Raman spectroscopy measurements to study the interaction between the materials, aiming at optimizing the active material utilization and the electrical conductivity.Then, the reference electrodes were printed onto the Celgard2500 separator and positioned between the active anode (graphite) and cathode (NMC622) in full pouch cells of 3 cm², as shown in Figure 1. Finally, 3-electrodes cells were electrochemically characterized performing galvanostatic charge and discharge (GCD) cycles at different C-rates and EIS measurements at different cell States of Charge (SoCs). The obtained results indicate that our novel printed reference electrodes do not alter the pouch cell operation and can be used to accurately monitor distinctively the potentials and the impedances of the battery electrodes.



Figure 1. On the left, a sketch of the three-electrode pouch cell configuration. On the right, GCD curves at C/5 measured for the three-electrode pouch cell using the printed reference electrodes: (a) LFP-D and (b) LTO-D. The letter D indicates 65% wt. of active material relatively to the solid content of the electrode materials.

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Integration of Temperature and Pressure Sensing Functionalities into Li-ion Pouch Cell on an Industry-Relevant Scale

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As part of the BATTERY 2030+ research initiative, the project SENSIBAT focuses on developing smart sensing functionalities, novel battery management system strategies, and state determining algorithms considering economic and environmental aspects. With the help of these sensors, integrated in Li-ion pouch cells, it is aimed to gain a better understanding of the battery during its operation.

Profound knowledge about the actual cell conditions (state-of-charge, state-of-health) during cycling can be used for a better prediction of the cell behavior. Indicators for possible degradation processes and failure mechanisms can be determined and enable a more accurate control of the cells in a battery pack, leading to improved BMS state estimation functions. That way, a significant increase in safety, lifetime and quality is targeted. The introduction of sensors into pouch cells is currently not done at industrial scale and therefore several problems can arise. One of them is incompatibilities during integration of the sensors during the pouch cell assembly process. Especially at the sensor feedthrough, it needs to be ensured that no electrolyte leakage appears, and the tightness of the pouch cell is given. Additionally, an interference between sensor and cell components, which can cause side reactions and unwanted by-products, should be avoided, as this can negatively influence the performance of the cell [1, 2, 3].

This work explains how the integration of the developed temperature and pressure sensing functionalities was conducted on an industry-orientated scale. A special focus within the SENSIBAT project is how the implementation influences the overall cell performance compared to equivalent reference cells without additional sensing elements.

A research pilot line was used to fabricate the Li-ion pouch cells with a nominal capacity of 5 Ah per cell. NMC622 cathodes and graphite anodes were stacked by using an automatic single-sheet stacking unit under dry-room conditions. To gain valuable insights and comparable data on how the conducted integration process influences the overall cell, a comparison of cells with and without integrated sensors was conducted. Therefore, a cycling test plan containing symmetric and asymmetric full cycles at different C-rates, pulse test sequences and electrochemical impedance spectroscopy analyses was performed.

The SENSIBAT project partners were able to exhibit that the sensor implementation did not negatively influence the electrochemical performance of the cells compared to the reference pouch cells. The absolute discharge deviation of the cells with and without embedded sensors is below 1%. Additionally, no major differences in the calculated pulse resistance values and electrochemical impedance spectra occur.

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Phase separated polymer electrolytes for Li-ion batteries using oligomeric carbonates

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In a variety of novel battery technologies, the development of electrolytes with high structural robustness while still maintaining uncompromised ionic conductivity. One such technology, is structural battery composites. To achieve the required electrolyte properties a two-phase system is used, where a liquid phase containing mobile ions permeates a stiff, mesoporous thermoset. These solid bicontinous electrolytes (SBE) are made through a process called polymerization induced phase separation (PIPS), in which a dimethacrylate monomer is dissolved in a liquid electrolyte and then thermally cured to form a solid. As it cures, the polymer becomes insoluble in the liquid electrolyte, creating the porous structure. By adjusting the amounts and structure of each component, the properties of the resulting material can be fine-tuned. [1]

Previously, the effect of changing monomer structure has been previously investigated, but little work has been done on systematically investigating the effect of the structure of the liquid electrolyte used in these systems. In this study, we explore how changes in the structure of the liquid electrolyte affects the phase separation process and in-turn the properties of the SBE. Oligomeric linear carbonate molecules of increasing lengths have been explored as the mobile phase in the SBE. By increasing the length of the linear carbonates, the thermal stability of the SBEs were greatly improved. In addition, the pore size could be increased, lowering the tortuosity of the SBEs. It was also found that the inherently low ionic conductivities of the oligomeric carbonates became the limiting factor of these systems. [2]

Vinnova via the Batteries Sweden competence center is acknowledged for funding this project.



Figure 1. Schematic of the phase separated electrolytes and the parameters that are varied

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ACCELERATING THE DISCOVERY OF ORGANIC BATTERY MATERIALS: FROM ATOMISTIC MODELLING TO ARTIFICIAL INTELLIGENCE

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The organic electrode materials (OEM) are emerging as a promising alternative to develop greener and sustainable battery technologies. However, significant improvements are still required in their cycling stability, rate capability and energy density. This can only be achieved through a fundamental understanding of the electrochemistry at molecular level establishing the structure-properties relationships. To contribute to this end, we are developing methodologies based on evolutionary algorithms (EA) and artificial neural networks (ANN) at interplay with density functional theory (DFT). The EA has initially been employed to predict the structure and electrochemistry of a set of dicarboxylates. In a second stage, we have developed a wider database of organic materials for energy applications that contains information about molecular geometries and high-level features extracted from DFT calculations. Based on this database, we have developed a machine learning approach to predict the redox potentials by giving only chemical species and molecular structures, completely by-passing the computer-demanding DFT calculations. A number of learning algorithms based on ANN have been investigated along with different molecular representations. Here, we have also included a layer to predict redox-stable compounds. This machinery has been employed to screen a large organic materials library (45 million molecules) leading to the discovery of novel cathode materials [1], which is actually one of the bottlenecks on the development of organic batteries. The computational materials design platform developed here has the potential of significantly contribute to accelerate the discovery of organic electrode materials with superior properties.

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INSTABAT sensibat



FIBRE OPTICAL SENSORS FOR OPERANDO MONITORING OF **INTERNAL PROCESSES IN LI-ION AND Na-ION BATTERIES**

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Insplorion's fibre optic sensors enable operando probing of physicochemical processes occurring inside lithium-ion and sodium-ion battery cells. The sensor probe is inserted between the separator and one of the electrodes and monitors processes in/on the electrode material such as plating, ion intercalation and capacity fading. The optical data is measured and collected using an Insplorion M8: 8-Channel Analyzer instrument (Figure 1), with which up to eight fibre optic sensors can be measured simultaneously. In this presentation we will give an overview of Insplorion's fibre optic sensing technology with several application examples showing how it can be used in research and development.



Figure 1. Insplorion M8: 8-Channel Analyzer can be used to measure on up to eight fibre optic sensors simultaneously.













INSTABAT smart multi-sensor platform

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An accurate and reliable knowledge of the in operando key parameters of a Li-ion battery is essential for its optimal use, safety and extended lifespan. Within the framework of BATTERY 2030+ initiative [1], the ambition of INSTABAT project is to monitor these parameters in order to provide higher accuracy in cell state indicators. INSTABAT partners has developed a proof of concept of physical (optic fibers, reference electrodes) and virtual sensing technologies and functionalities [2], [3]. The smart cell should be able to perform in operando monitoring of temperature and heat flows, Lithium concentration, CO2 concentration, absolute impedance, electrode potential and polarization. Multi-sensor platform challenges are to interface successfully these sensors, which – combined with the appropriate BMS – is able to improve the accuracy of the SoX cell indicators estimators.

To build the platform, it is necessary to find a target hardware able to measure the signals coming from our sensors but also to process them to feed the virtual sensor models and the battery state estimation algorithms. INSTABAT sensors are low TRL and require specific non-integrated instrumentation and lab equipment to acquire their signals. In addition, the selected target must avoid any strong constraints on algorithms and model developers in terms of computational or memory resources. Consequently, the platform is based on an instrumentation computer with PXI modular architecture using LabVIEW software engine.

The host software (Figure 1) realizes the following tasks:

- control/command measurement devices to acquire usual BMS sensors and INSTABAT sensor signals,
- pre-process signal to extract battery parameters (ex: temperature from OF spectrum),
- operate virtual sensors algorithm (Electrochemical model, Thermal model) and BMS state indicators computations compiled in a dedicated library
- and finally perform time synchronization and log all the data produced by the platform



Figure 1. POC multi-sensor platform architecture

The platform is currently operational for the INSTABAT project cycling and abusive tests and is being completed or updated as soon as a new sensor or a new version is available.

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Hybrid polymer-liquid lithium ion electrolytes: effect of porosity on the ionic and molecular mobility

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Lithium ions batteries (LIB) are the most prominent technology in the field of energy storage where liquid electrolytes are the most commonly used solution in the battery industries. Despite their attractive properties (such as high ionic conductivity and thermal stability at the ambient/sub ambient conditions), they have shown safety concerns due to their flammability which has led to the development of new electrolytes systems.

An emerging field are hybrid electrolytes (HEs) which are defined as electrolytes composed of at least two well-defined phases. One of the phases (or even both) conducts the ions and the other phase lends mechanical stability. A promising example of HEs are solid-liquid electrolytes such as the structural battery electrolyte (SBE ¹) where two discrete co-existing phases are formed: one thermoset structural phase providing mechanical integrity and one percolating liquid ion-conducting phase. The phase separation is possible as a result of the variations in the solubility parameters of the monomers with respect to those of the formed polymers. The main feature of the polymer network is the microporous structure that gives structural integrity to the system thanks to the polymeric solid phase and, at the same time, conducts the ions through the percolating liquid phase. Although the SBE has shown remarkable properties results when tested in a negative half-cell lamina ², it is not fully understood how the morphology and chemical composition affect the molecular transport in the system.

The present work investigates ions transport in a series of hybrid solid-liquid electrolytes with different liquid contents using NMR-techniques coupled with morphological and electrochemical analysis (Figure 1). It is clearly shown that not only the tortuosity but also the ions conductance through the polymer phase plays a critical role in determining the electrochemical performances ³.



Figure 1: Figure illustrating the interactions of the different electrolyte species with the polymer wall.

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The GigaGreen Project. Towards the sustainable giga-factory: developing green cell manufacturing processes

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Horizon Europe GigaGreen Project [1] aims to develop a greener and more scalable cell production technology aimed to the industrial level following a Design to Manufacture (DtM) approach, with the ultimate goal of making Europe a strategic leader in the Li-ion battery production. In this line, GigaGreen focuses on the increment of the cost-efficiency and safety of processes and products, for example, one of the most important steps of this project is to move from Polyvinylidene Fluoride (PVDF) as binder, which requires the organic, toxic and expensive solvent N-Methyl-2-Pyrrolidone (NMP) to more sustainable and economical water-processable Fluorine-free binders. The importance of this improvement is related to the high costs of electrode processing, from mixing to deposition, which represents nearly 40% of the cell manufacturing costs [2].

The role of Politecnico di Torino (POLITO), coordinator of the GigaGreen project, is to develop a Si/C compositebased wet anode, starting from laboratory scale and scaling up to a small pilot line. In particular, the challenge is to optimize the slurry preparation by studying how the rheological parameters can influence the coating step, in order to maximize the yield production for a promising anode active material. The so obtained anode electrodes present a higher ratio of Si compared to commercial ones and so higher specific capacity can be obtained.

To reach the project goals, an in-depth characterization of the operating parameters of the roll-to-roll coating machine is been carried out in POLITO, producing standard anodes with commercial graphite (Figure 1).

The presentation will show that one of the most critical parameters is the gap imposed between rolls during the slurry deposition: this crucial parameter is directly related to the quantity of active material on the electrode and its final density. The speed of deposition and the oven temperature during the drying process are other parameters that can influence the quality of the slurry having a significant effect on the final product. It is very important to balance all of these parameters so that the overall process can be more energy and cost-efficient than the actual one utilized at industrial level.



Figure 1 – Anode coating on roll-to-roll machine

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Raman spectroscopy of NMC and first principles study of Li_xNiO₂ cathodes for Li ion batteries

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A better understanding of the cathode active materials based on Ni-Mn-Co-oxides plays a crucial role in the improvement of lithium-ion batteries. The assessment of the structural order in LiMO, (M = Ni, Mn, Co) by XRD is difficult to achieve, due to the close positions of the characteristic peaks. However, Raman spectroscopy would help in this task, providing an easiest way to identify the presence of orthorhombic and spinel phases in the cathode materials. Complementary, calculations of the equilibrium structure of some cathodes containing Li at different percentages have also been performed. Since the dominant transition metal both in the (811) core and in the (631) shell of the core-shell NMC cathodes used in BAT4EVER project is nickel, we have deeply investigated LiNiO₂ lithiated structures in the layered R-3m structure. Atomistic simulations of the battery materials can shed light on those properties of the materials difficult to assess experimentally.

In this work, we report the different phases identified in the cathode materials provided by the BAT4EVER partners by means of Raman spectroscopy, as well as the study of the change in the structural, electronic and magnetic properties of Li_xNiO_2 at various Li concentration x within the first principles density functional theory (DFT) framework. The analysis of the Density of States hints to the formation of a band gap in agreement with the experiment, where an insulating behavior with a gap of 0.5 eV was measured, but never found before in calculations of LiNiO₂ in the R-3m structure. The analysis of the formation energies of various configurations of Li_xNiO_2 found that the total energy is highly sensitive to the arrangement of the Li vacancies.



Figure 1. Structure of LNO in the hexagonal R-3m space group with 192 atoms unit cell.

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Challenges and opportunities for Copper hexacyanoferrate in rechargeable aqueous Zn-ion batteries

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Copper hexacyanoferrate (CuHCF) is a typical Prussian Blue Analogue (PBA) compound that is interesting for ion insertion thanks to its open structure with cubic symmetry and large cavities that can host several cations (e.g. alkali metal ions, divalent cations). This has fostered researches on CuHCF as possible cathode in aqueous Zn-ion batteries (ZIBs) with a mild pH, which could constitute a prospective cost-effective and safe rechargeable technology for stationary storage of electricity [1, 2]. Aqueous Zn/CuHCF cells have intrinsically a limited energy density (\leq 100 Wh·kg⁻¹), however, their power delivery is excellent and thereby can amply sustain high C-rates, while CuHCF undergoes only minor volume variations upon cycling [3]. Moreover, limited environmental impact, non-flammability and wide abundance of the constitutive elements make these ZIBs attractive for storing intermittent electricity produced via renewable sources [4]. Aside the difficulty of stabilizing the metallic Zn interface in mildly acidic solutions and enhancing its utilization [4], the main obstacle to their development hinges on mitigating a pronounced ageing of CuHCF upon cycling [5], which manifests through progressive appearance of a plateau on charge around 1.8 V vs. Zn²⁺/Zn and is accompanied by capacity fading (Figure 1).

So far, the CuHCF ageing mechanism in ZIBs has remained elusive and only some speculative attempts have been made to explain it by a possible phase segregation and generation of new non-stoichiometric Zn-rich phases (e.g. $Zn_xCu_{1-x}HCF$) [5-7], while also signs of Cu dissolution from CuHCF were noted [8], yet thought to be marginal. Here, we will discuss that CuHCF is not as stable as previously thought and we will show that the Cu dissolution issue is linked to its ageing mechanism. The latter was investigated via a thorough study employing various *ex situ* and *in situ* analyses [9]. We will show that the Cu dissolution from CuHCF is spontaneous, that it occurs at the particle surface and that it causes a concurrent, gradual activation of the Fe³⁺/Fe²⁺ couple, while the formed Cu vacancies can be filled by the Zn^{2+} ions. These insights into the CuHCF aging process may help in devising strategies to mitigate this crucial aspect and thus improving effectively the cycle life of these ZIBs.



Figure 1. Schematic view of a Zn/CuHCF cell and voltage profiles at ≈8C with a 1 M ZnSO₄ electrolyte.

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Modeling self-healing binders for silicon anodes

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Silicon anodes typically suffer from poor intrinsic conductivity and dramatic volume change during charge/discharge cycles, leading to surface cracks and, eventually, to anode pulverization. A promising way to overcome these failures is to embed the silicon particles in a conductive self-healing binder. In the EU project Bat4ever, autonomous self-healing is introduced through silicon polymer-coated particles to be implemented as anodes in the self-healing batteries. Atomistic first-principles and molecular dynamics simulations have been carried out to study self-healing B-OH-PANI and PVA monomers and dimers and their interaction with silicon surfaces. We have derived the lowest energy configurations of the monomers and dimers and studied their mutual interaction, which leads to a large number of dynamic hydrogen bonds (see figure). The study of the interaction of the monomers with silicon surfaces has revealed both the formation of surface bonds and longer range electrostatic interactions. The co-adsorption of B-OH-PANI and PVA monomers.



Figure 1. B-OH-PANI and PVA monomer configurations from Molecular Dynamics Simulation. The red dotted lines indicate the hydrogen bonds

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Automated electrolyte formulation and coin cell assembly for highthroughput lithium-ion battery research

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Battery assembly and evaluating the performance of batteries with new chemistries are processes in the battery research workflow that can be time-consuming and may result in large cell-to-cell variations, which can negatively impact the accuracy of the results obtained. Automation is one type of accelerator to address these challenges and improve the reproducibility in battery research.

In this context, ODACell [1], our automated robotic setup, has been developed to enhance the rate of testing and reduce the variation of results due to human error in battery research. Specifically, ODACell is a new automated setup rivaling other published robotic setups, like Clio by Dave *et al.* [2], AutoBASS by Zhang *et al.* [3], and Poseidon by Svensson *et al.* [4], that can assemble Li-ion battery cells, and it is uniquely equipped for combinatorial experimentation; the system combines electrolyte formulation, batch coin cell assembly, and cycling into one setup, allowing for high-throughput electrolyte screening along with Li-ion coin cell assembly.

Using LiFePO₄||Li₄Ti₅O₁₂-based full cells with dimethyl sulfoxide-based model electrolyte, the automated setup was able to assemble 131 coin cells, with a conservative fail rate of 5%. Additionally, the relative standard deviation of the discharge capacity after 10 cycles was 2%. Moreover, the system was also used to investigate the influence of added water in the model electrolyte on cycling performance, which found overlapping performance trends between coin cells with 2 vol% and 4 vol% of water in the electrolyte.

Overall, ODACell has the potential to be a useful tool for advancing battery research by enhancing the rate of testing and reducing the variation in results. While there are other robotic systems besides ODACell for battery materials acceleration, its unique combination of robots incorporated in the robotic setup allows a broader set of tasks to be automated.



Figure 1. ODACell, an automated robotic setup for electrolyte formulation and battery assembly.

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Generating novel electrolyte-systems is of urgent need, for batteries as well as for supercapacitors acting as short-time power-storage devices. While solid electrolytes offer promising alternatives to conventional liquid electrolytes, they undergo irreversible failure during cycling. Intrinsic self-healing materials ^[1] based on dynamic bonds are suitable candidates as alternative electrolytes ^[2], since reversible bonding can compensate failure of the materials consequently extending the lifespan of a battery.

We here report on the use of supramolecular and dynamic covalent bonding systems to embed selfhealing ^[3] and vitrimeric properties ^[4] into electrolyte-systems, requiring fundamental knowledge about bonding strength and dynamics in highly polar and even ionic-liquid environment. We have focused on two different bonding systems, one composed of hydrogen bonding-systems; the other of covalent dynamic bonds, enabling vitrimeric exchange during charge-transport through the electrolyte-medium. Additionally, mechanical properties of poly(ionic liquid)s were reinforced by covalent crosslinking and ionic conductivity was enhanced by incorporating ionic liquid/lithium salt mixture into polymer network (forming ion-gels). A critical factor is to maintain the dynamic feature in the temperature window of interest, still keeping the required ion-conductivities intact. The materials we are reporting herewith not only suffice these requirements, but also allow to embed self-healing properties into the final (solid) material. Furthermore, we demonstrate the 3D-printability of vitrimer-based electrolyte-composites ^[5].



Figure 1. Schematic representation of self-healing mechanism.

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Loss of charge capacity in lithium-ion batteries stem from different phenomena, one of which is mechanical degradation. In this study the mechanical properties of a positive electrode layer are investigated using the discrete element method (DEM) in order to link the local mechanical behaviour, on the active particle scale, to the global behaviour of the electrode active layer. Grasping the coupling between length scales is crucial for understanding and mitigating the mechanical degradation phenomenon and as the active particles form a granular structure in the electrode layer, DEM is a well-suited method to apply. The DEM model developed considered both interaction between active particles, as well as interaction between particles separated by binder. This study targeted to replicate the determined in-plane unloading stiffness of the electrode layer, which had been measured experimentally by Gupta et al. [1] through a U-shape bend test. The model was able to capture the constant stiffness in tension at all strain levels and the stiffness at increased load rates, could be captured quantitatively by increasing the binder stiffness. This work lays an excellent base for further investigations of the mechanical properties of the active layer and its mechanical degradation mechanisms, such as swelling and fracture of the active particles.



Figure 1. a) The representative volume element used when analysing the in-plane mechanical loading, b) simulation results of the in-plane unloading stiffness compared to experimental results.

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MY RESEARCH ACTIVITY WITH KALIUM

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Potassium-ion batteries (PIBs) are one of the top candidates to replace Li-ion batteries for stationary applications. Li-ion batteries (LIBs) have reached unprecedent targets of performance and safety, which ensure the Li-ion system as the best choice for portable divices and electric vehicles. Nevertheless, as lithium is now in the list of critical raw materials due to its low abundancy (0.0017 wt% in the Earth crust) alternatives are coming on the scene. An interesting element to replace lithium in batteries is kalium, which is abundant on Earth (2.09 wt%), evenly distributed and characterized by a very low standard equilibrium potential (-2.93 V vs. SHE with respect to -3.09 V vs. SHE of Li⁺/Li) and Lewis acidity (smaller solvated ions and thus faster conduction). Nonetheless, K-ions batteries show lower volumetric and gravimetric energy density with respect to LIBs, but still they can be a good alternative for stationary storage enabling renewable energy use in the electricity grid and reducing the impact on future lithium needs. Even if this technology is receiving increasing attention from the research community, among all the post Li-ion systems K-ion batteries are welcomed with some perplexities. Indeed, even if I can count very limited research experience, the most asked question to me is the simplest: "Do they really work?". Yes, they actually do. As a matter of facts, my contribution is meant to show some results achieved during the last 2 years of my research activity and which is now the main topic of my PhD thesis. Here I am presenting an in-depth electrochemical characterization on commercial carbon anodes for K-metal batteries which allowed us to get insights on the storage mechanism of bigger K-ions which suit better amorphous structures; K-ions were found able to insert into both amorphous and anatase TiO₂ nanotubes with promising capacity retention; many polymer electrolytes [1,2] were found suitable to guarantee in K-ion systems high ionic conductivity, homogeneous ions transference and stable interfaces for long cycling results. Among them a Kraft lignin matrix crosslinked with poly(ethylene glycol) diglycidyl ether provided glorious stability at the potassiummetal interface, allowing to reach 800 stable and performing cycles. Furthermore, knowing in advance their final use, we have the chance to already design PIBs for large scale commercialization to be sustainable and low cost. In light of this consideration, as well as for the above-mentioned electrolyte, a highly porous carbon material has been successfully synthetized starting from the sustainable and low cost lignin and employed as anode for potassium-metal batteries. But what can be done next to improve this technology that is in its infancy?

To conclude, these results may represent the validation of all the kalium premises as the perfect lithium allay toward the energy transition and the encouragement for increasing future studies on K-ion batteries.¹



Figure 1. Cycling performance of SuperP/lignin-based electrolyte/K-metal half-cell.

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Development of an ORP-EIS sensor for in situ SoX determination

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Lithium ion batteries (LIB) are used in many applications for energy storage, ranging from mobile devices to electric vehicles. A lot of research is performed with the aim of developing more environmentally friendly and safer batteries with better performance, including longer life. One way of improving performance and lifetime of a battery is by creating sensors that are capable of monitoring the state of a battery cell module in real time. Using these sensors, the start of degradation and failure mechanisms can be detected before a loss of performance occurs. This information can be used as an input for a battery management system (BMS) that can make decisions on the best operating and charging conditions for each individual battery in the module.

Odd Random Phase multisine Electrochemical Impedance Spectroscopy (ORP-EIS) has proven to be a powerful technique to characterise LIB [1]. The impedance response of either the charge transfer reaction on the positive electrode or the solid electrolyte interface can provide valuable information regarding the state of health (SoH) and state of charge (SoC) of the battery cell. Due to the specifically designed signal, ORP-EIS also provides information on the stochastic noise levels, non-stationarity, and non-linearity of the system, which can be used to determine the accuracy and validity of the measurement. These characteristics make the ORP-EIS technique interesting to use as sensing technology for BMS.

In this work, a sensor is designed to perform ORP-EIS measurements on commercial grade battery cells. It is designed to be a standalone unit, capable of the application of the ORP-EIS signal, data acquisition and data processing through an embedded processor. It will operate with an advanced BMS for the in situ identification of the SoH and SoC of a battery cell stack. The battery cells under study are commercially available and use NMC 811 and graphite as positive and negative electrodes, respectively. Their internal impedance is very low (m Ω range), see. Figure 1. This means that the signals are easily distorted by external influences, and provides an additional challenge to obtain accurate readings.



Figure 1. ORP-EIS data of commercial Kokam cell collected using the developed sensor.

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FIBER OPTICAL DETECTION OF LITHIUM AND SODIUM PLATING IN INTERCALATION BATTERIES

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Plating of metallic lithium or sodium is one of the most critical events causing problems in modern intercalation batteries. The plating on the anode, for example as a result of a too high charging rate, causes detrimental side reactions leading to a reduced lifetime of the battery. The growth of lithium or sodium dendrites can also lead to catastrophic failure as they can penetrate the separator and cause a short-circuit in the cell. This presentation focuses on recent findings from Uppsala University, where information from a fiber optical sensor inside a battery was found to reveal early signs of plating [1,2]. Figure 1 below shows an illustration of the fiber on top of the hard carbon anode in a sodium ion battery, and this type of experiment could eventually provide a battery management system (BMS) with input to optimize the charging rate just below the limit of plating.

Having access to a sensor inside the cell on top of either the anode or cathode thus offers unique possibilities to track detrimental reactions in the battery. We also anticipate that the fiber optical sensor could serve as a research tool to learn more about the intercalation and plating mechanisms, as well as the optical properties of the anode or cathode materials during cycling [3]. Preliminary experiments on a prototype commercial sodium ion battery also indicated that the plating could be detected via the fiber while it was not clearly seen in the cell voltage, even if a reference electrode was included in the cell. Comments will also be made on future applications of this type of sensor. The small size of the optical fiber allows it to be positioned at specific spots in a large battery cell. This is, for example, advantageous as the plating in commercial cells often can be heterogeneously distributed.



Figure 1. Schematic picture of the optical fiber on top of the anode, and the possibility to feed information to a BMS.

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A holistic approach on the feasibility of garnet-based all solid-state lithium batteries

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Recent technological developments in battery science have allowed a widespread growth of both electronic portable devices and electric vehicles (EVs). Much larger sizes of the EV batteries raise new concerns about safety of the electrolytes used in such cells, and hence numerous research efforts are dedicated to minimising flammability or directly removing the organic liquid electrolytes commonly used in lithium-ion batteries.

Inorganic solid-state electrolytes (SSEs) are ceramic and glass materials able to conduct ions. Among many formulations available, garnet $Li_7La_3Zr_2O_{12}$ (LLZO) is the most promising oxide phase. Its unique lattice supports a high Li-ion conductivity, while keeping desirable features for both the electrochemical stability window and overall air stability-processability. Such characteristics should be indeed favourable to tackle the flammability problems previously mentioned. However, a number of critical issues emerge when moving from a technology based on a liquid infiltrating the electrodes to a solid being sandwiched in between them, instead.

In this poster, we present the research carried at Uppsala University to improve these SSE materials for possible future commercial applications. These SSE materials need improvements at the compositional level, as it is known that their crystallographic and ion-conductivity properties will directly depend on the elemental substitution of the atoms forming the lattice. We consider these important features for the often-neglected Lanthanum sites. Another aspect to improve is the formation of solid materials that can be used in actual electrochemical systems, focusing in this case on how to press/consolidate pellets of pure LLZO powder (uniaxially or isostatically) and on how to ease their sintering and final densification. As a last crucial improvement, the surface of these SSEs needs to be functionalised to achieve their best possible performance. We will present a boron-based surface treatment that is expected to both promote the surface affinity with lithium and neutralise detrimental carbonate formation. We will as well analyse the influence of the surface treatment at the interface level, and its actual effect on the assembly of functional all-solid-state batteries.



Figure: Visual demonstration of increased lithiophilic character of surface treated pellets (on the right) compared to atmosphere exposed pellets (down left)









In-Situ Liquid-State NMR Investigations of Lithium-ion Battery Electrolyte Decomposition

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Liquid electrolytes play important roles in the lithium-ion batteries (LIBs). In particular, an amount of the electrolyte decomposes to form solid-electrolyte interphase (SEI) that stabilizes the electrolyte-electrode interfaces, while the remining bulk solution transports the cation between the electrodes. In order to develop better electrolytes such as with improved safety and chemical stability, efforts have been devoted to understanding the electrolyte decomposition process, which are mainly performed by studying the solid products that precipitate in the SEI or gases that are released during the decomposition. However, the liquid products or species that are soluble in the electrolyte remain as a mystery. Here, we employ in-situ liquid-state nuclear magnetic resonance (NMR) spectroscopy to study the evolution of LIB electrolyte composition caused by the degradation process. Using 1D and 2D NMR techniques, we confirm that some degradation products are indeed soluble in the electrolyte. The identification of these compounds gives insights into the degradation processes, which also has implications on how the long-term function of the electrolyte will be affected. Besides the new insights into electrolyte decomposition process in the LIBs, the presented techniques can be extended for studying electrolytes in a broad range of battery systems.

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OCV HYSTERESIS IN NIMH – A STRUCTURAL INVESTIGATION

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The nickel metal hydride (NiMH) battery is a well-established battery type that started out as a lighter and less toxic alternative to the nickel cadmium battery. Today it used both for hybrid electric vehicles, such as the Toyota Prius, and stationary energy storage. One phenomenon that affects the use of NiMH battery is Open Circuit Voltage (OCV) hysteresis. OCV hysteresis is when the OCV of a battery differs depending on the charge/discharge history, Figure 1. OCV hysteresis has been recorded for materials that undergo phase expansion during a charge cycle, such as Ni(OH)₂ and LiFePO₄. The hypotheses on the origin of the OCV hysteresis all concern phase changes but disagree on the exact mechanism. **[1]** Furthermore, little is known about the origin of OCV hysteresis in the Ni(OH)₂ electrode, although electrochemical techniques have been used to study it. **[2]**

This study has investigated the $Ni(OH)_2$ electrode-material at 50% State of Charge (SOC) at two different hysteresis states using several characterization techniques: XRPD, EXAFS (on Ni, Zn, and Co), Raman, and Neutron diffraction. Differences are found that can be related to the OCV hysteresis behavior.



Figure 1. State of charge as a function of OCV, with impact of hysteresis, for NiMH cell.

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SELF-HEALING POLYMER INTEGRATION INTO CORE/SHELL NMC CATHODE MATERIAL

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Li-ion batteries are prone to the failure mechanisms because of drastic structural changes, degradation and finally loss of functionality caused by thermodynamic, chemical, and mechanical instability of materials. These degradation processes in the battery cells can be minimized or avoided through the preventing approaches, for instance by using so-called self-healing materials – materials that recover battery functionality after mechanical damage, chemical deterioration or properties changes [1]. Recent studies have shown that selfhealing systems can enhance significantly the lifetime of battery materials relying on the improvement of the mechanical characteristics and battery cycling stability [2-3].

The aim of the present work was to investigate the effect of the self-healing functionalities on the electrochemical performance of the Lithium-Nickel-Manganese-Cobalt-Oxide (so-called NMC) based cathode materials. For this purpose, Ni-rich Core/Mn-rich shell cathode particles have been synthesized by means of cost efficient and easy process-controlled co-precipitation method. As precursors, aqueous solutions of the Li, Ni, Mn and Co salts have been employed in the required ratio. The co-precipitation of the precursor solution has been performed by dropwise addition of the oxalic acid solution under continuous stirring with following drying and heat treatment of the obtained precipitate. For achievement of core and shell in different compositions, two-staged synthesis approach has been applied.

To study the influence of the polymer binder on the electrochemical performance of the synthesized NMC particles, battery half-cells have been produced using two different binders – PVDF binder and PANI/PVA-Borax self-healing polymer (SHP). Results of the electrochemical impedance spectroscopy have shown the lower charge transfer resistance of the SHP-integrated sample compared to the sample, containing PVDF binder. Initial galvanostatic charge/discharge results demonstrated that PVDF containing NMC sample leads to a higher first cycle capacity than SHP-integrated powder. However, the initial coulombic efficiency loss of SHP sample was 60 mAh/g lower than of PVDF sample in first cycle, proving the higher efficiency of the SHP sample characterized by the cycling test. After the formation procedure both electrodes showed similar specific capacity. But the NMC-PVDF electrode has lost sharply its capacity after 400 cycles, while the NMC-SHP electrode has continued to work with minor capacity reduction.





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ENHANCED PERFORMANCE OF LI-ION BATTERY ELECTRODES PROTECTED BY ATOMIC LAYER DEPOSITED ULTRATHIN FILMS

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Protective surface coatings or electrolyte additives can be employed to prevent uncontrolled growth of the solid electrolyte interphase and enhance the performance of the Li-ion batteries. In our approach, we have focused on the surface modification of the Li-ion electrodes by atomic layer deposited ultrathin films. Our contribution describes the performance of the silicon-graphite based anode covered by ZnO films and LiFePO₄ cathodes protected by Al₂O₃ layers.

Thin ZnO and Al_2O_3 films were prepared by atomic layer deposition (ALD) using diethyl zinc and trimethyl aluminum as precursors and water vapors as reactant. The deposition was carried out at 100 °C with a modified deposition recipe for porous substrates. The estimated growth rate was about 0.1 nm per ALD cycle.

The silicon-graphite based anode was prepared by mixing 80 wt% silicon-graphite (ball milled at 20:80 silicon/graphite weight ratio), 10 wt% of carbon black, and 10 wt% of sulfonated-alginate as a binder. Galvanostatic charging/discharging characterization of the silicon-graphite anode was performed in a coin cell configuration against Li/Li⁺ electrode in the voltage range 0.01-1.5 V using C-rates from 0.05 up to 2. At the c-rate=2, the silicon-graphite electrode protected by 20 cycles of ZnO (approximately 2 nm of thickness) showed a capacity of 500 mAh/g which is nearly 5 times higher value compared to the unprotected pristine anode. After 100 charging/discharging cycles at c-rate=1 ZnO protected anode exhibited 1.5 times higher capacity than the uncoated one. The better performance of the ZnO-covered silicon-graphite electrode was corroborated by electrochemical impedance spectroscopy. The impedance analysis revealed lower impedance values for the solid-electrolyte interphase and charge transfer components of the ZnO-protected silicon-graphite anode. ZnO is known as an active anode material, therefore its application as a thin film increases the capacity and protects the silicon-graphite anode against electrolyte at the same time. ZnO exhibits relatively high lithium storage capacity (987 mAh/g) and high volume expansion under lithiation. Consequently, ZnO coverage can follow the volume changes of the silicon-graphite anode during lithiation and delithiation. In addition, ZnO protecting layer increases the transfer of Li-ions at the solid-electrolyte interface.

ALD-grown Al₂O₃ films were selected for the protection of the LiFePO₄ cathode. A commercial cathode (NANOMYTE BE-60E (NEI Corp.)) with a thickness of 70 μ m was used. Charging/discharging experiments in the half-cell configuration revealed that a decrease in the discharge capacity at c-rate=2 can be compensated by protecting ALD layers. The cathode covered by 5 ALD cycles of Al₂O₃ (0.5 nm) showed a discharge capacity of 120 mAh/g compared to 40 mAh/g for the unprotected pristine cathode. In the full cell configuration, using graphite anode, the LiFePO₄ cathode covered by 20 cycles of Al₂O₃ (2 nm) exhibited a capacity of 120 mAh/g compared to 50 mAh/g obtained by the unprotected pristine LiFPO₄ cathode. The improved discharge capacity of the Al₂O₃-protected cathode was retained also after 100 charge/discharge cycles at c-rate=1. The capacity of the covered cathode after 100 cycles was still 120 mAh/g, while the unprotected pristine cathode was confirmed by the impedance spectroscopy, showing lower charge transfer impedance for the Al₂O₃-covered cathodes. Al₂O₃ ultrathin layers on the LiFePO₄ cathode prevent direct contact of the electrode and electrolyte, suppress side reactions, inhibit dissolution of the cathode component, and enhance Li-ion transfer through the interface at the same time.

In conclusion, protection of the Li-ion battery electrodes by ultrathin ALD layers can be considered as an effective way for improving rate performance and cyclability, particularly at high charging/discharging rates. Modification of the electrode surface by ALD layers resulted in the formation of the solid-electrolyte interphase layer which is more compact and stable.

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Non-flammable localized highly concentrated electrolyte for lithium-ion batteries

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One major shortcoming of current lithium-ion batteries is the flammability of organic liquid electrolytes. Therefore, there is an interest to design non-flammable liquid electrolytes. An emerging concept within this research field is the development of localized highly concentrated electrolytes (LHCEs).¹ This type of electrolyte is based on the concept of highly concentrated electrolytes (HCEs), but possesses lower viscosity, improved conductivity and reduced costs due to the addition of diluent solvents. In this work, two different hydrofluoroethers, i.e., bis(2,2,2-trifluoroethyl) ether (BTFE) and 1,1,2,2-tetrafluoroethyl 2,2,3,3tetrafluoropropyl ether (TTE), are studied as diluents in a phosphate-based non-flammable liquid electrolyte.² These two solvents were added to a highly concentrated electrolyte of 3.0 M lithium bis(fluorosulfonyl)imide (LiFSI) in triethyl phosphate (TEP) whereby the salt concentration was diluted to 1.5 M. Detailed insights into the solvation structures of the HCE and LHCE were obtained using complementary techniques of Raman spectroscopy and Nuclear Magnetic Resonance (NMR) spectroscopy. Furthermore, molecular dynamics simulations revealed that the highly concentrated Li⁺-TEP solvation sheath formed in an HCE can be shielded by the diluents TTE and BTFE in a LHCE. The simulations have helped clarify the energetic interactions among the components in the LHCE, which confirm the experimental findings from viscosity and NMR measurements. Operando pressure measurements reveal that the LHCEs analyzed in this study generate insignificant amounts of gas (< 10 mbar) in NMC622 graphite cells during formation cycling, while a cell containing 1.0 M LiFSI in TEP produces significant amounts of gas (450 mbar). The formation of gaseous products in 1.0 M LiFSI in TEP is accompanied by solvent co-intercalation and rapid cell failure, as revealed by operando XRD. This study provides insights into the solvation structure of LHCEs and highlights the connection between electrochemical performance and pressure evolution.



Figure 1. Overview figure of the main results i) reduced pressure evolution using LHCEs and ii) the different effects of the two diluents on the solvation structure

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Hard Carbon from Softwood Kraft Lignin for Sodium-Ion Batteries

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Lignin is the second most abundant natural polymer in plants' cell walls and an attractive carbon precursor due to its renewable source, low cost, and high carbon content.^{1,2} Efforts on the transition from petroleum-derived materials to sustainable materials and the fast-growing demand for energy storage devices created a unique opportunity for lignin as a bio-based carbon precursor. Lignin-based carbons have been studied for manufacturing anode electrodes in Li- and Na-ion batteries, and electrodes in supercapacitors.^{3–6} Properties of the precursor—such as purity—and conversion process can impact the properties of the resulting hard carbon and its performance. Conversion parameters and different pre-treatments or post-treatments of the materials are important for producing hard carbon with controlled morphology and optimized properties. Here, we used a high-purity softwood kraft lignin from the LignoBoost process for producing hard carbon. We studied the impact of different conversion parameters such as pre-stabilization and carbonization temperature on the carbon structure and morphology of hard carbon. In addition, we used different size reduction steps to control the particle size and surface morphology of hard carbon. The resulting hard carbons were tested as anode electrodes in Na-ion batteries.

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Understanding the mechanical properties of polymer electrolytes from atomistic simulations

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Self-healing polymers have caught much attention for potential applications in electrochemical energy storage systems because of their superior mechanical properties. However, unlike ion transport properties where much has been understood recently with the aid of atomistic simulations [1-3], the understanding of mechanical properties of polymer electrolytes at the atomistic level remains elusive. In this ongoing work, a model polymer electrolyte system, i.e., poly(ethylene oxide)-LiTFSI, was considered for a systematic study of the impact of molecular weight, temperature, and salt concentrations on mechanical properties, such as Young's modulus, storage, and loss modulus with both non-equilibrium and equilibrium molecular dynamics simulations. This work will provide a benchmark for computing the mechanical properties of polymer electrolyte systems and shed light on the molecular mechanism of self-healing polymers.

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Characterization of the degradation in realistic electrode microstructures using a coupled phase field damage model

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Key words: Lithium-ion battery cell, heterogeneous microstructural characteristics, active material particle, electro chemo-mechanical coupling, Modelling and Simulation, Phase-field damage, fracture.

Lithium-ion batteries (LIBs) have become a popular choice for energy storage systems due to their high coulombic efficiency and energy density. The secondary particles in the LIBs electrode materials are composed of numerous randomly oriented single-crystal primary active particles. The disintegration of these primary particles may cause structural instabilities and capacity fade, and a better understanding of these phenomena is therefore desirable. These particles can fracture as a result of both mechanical loading and chemical interactions within the solid. Modelling LIBs is a multi-physics challenge, as it involves considering the electro-chemo-mechanical phenomena and their interactions on different length scales. The volume changes of the active particles during electrochemical cycling create mechanical stresses, while the mechanical state of the battery provides a driving force for diffusion of lithium.

A numerical modelling framework is proposed to study the degradation of battery electrodes. This model combines mechanical and electrochemical processes to solve the nonlinear equations of surface charge transfer, lithium diffusion, and mechanical stresses. By incorporating phase field damage, the model tracks the evolution of crack growth and mechanical failure of the active particles. The coupled equations were solved in a finite element framework using COMSOL Multiphysics. The comparison of numerical results with experimental data shows that the model can effectively analyze particle cracking and mechanical instabilities, which have a significant impact on battery performance. Specifically, the model provides numerical results for both intergranular and transgranular fracture within the secondary active material particles. Exploring various factors that contribute to the degradation process offers opportunities to design advanced electrodes for high-performance Lithium-ion batteries.













HEATING ELEMENT ON THE POUCH CELL

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One of the main issues of Lithium Metal Batteries (LMB) is dendrite growth, which is one of the main causes of degradation. There is a number of research where preventing dendrite growth in LMBs is studied. Different self-healing methods for LMBs have been developed in the HIDDEN project. TILC [1] (i.e., thermotropic ionic liquid crystals) is one of the studied self-healing methods. This method is based on heating of the TILC electrolyte up to a phase transition temperature, during which lithium dendrites are destroyed. Self-regulating heating elements [2] allow temperature control without control electronics. Elements are based on positive temperature coefficient (PTC) materials allowing heat control between 0-80 °C or negative heat coefficient (NTC) ceramics suitable for temperatures higher than 100 °C.

Several heating elements were investigated to apply heat to a pouch cell. The screen-printed heating element can heat a pouch cell to 100 °C. The heater area is $35 \times 35 \text{ mm}^2$, as shown in Figure 1a. DC voltage was applied on the heating element and temperature was measured by a thermocouple, shown in figure 1b. Different temperature sensors have been used, such as thermocouples, and thermal cameras. To improve the thermal control of the heating element on the pouch cell HIDDEN collaborates with SPARTACUS. In this collaboration, SPARTACUS will investigate the thermal control of the heating element, and it will measure the temperature of the cell. Another heating element developed is a thin metal film which was retrofitted on a pouch cell. The heater area is $47 \times 47 \text{ mm}^2$, as illustrated in Figure 2.









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a)

Figure 2. Retrofitted heater on a pouch cell.

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IMPROVED ELECTROCHEMICAL PERFORMANCE ENABLED BY SOLUTION-BASED SYNTHESIS: CATHODES, ANODES, AND ELECTROLYTES

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Batteries have become ubiquitous in our modern society, finding their use in applications ranging from electric vehicles to stationary energy storage. Improving their functional characteristics relies significantly on the development of innovative chemical synthesis processes for electrodes and electrolytes. This work will highlight several instances where the IMO-Imomec group of UHasselt and Imec (Belgium) has used chemical approaches to advance the electrochemical performance and/or sustainability of existing and forthcoming battery chemistries.

The mining, refining, and processing of cobalt required for lithium-ion batteries (LIBs) has numerous negative societal and environmental consequences. Therefore, we conducted extensive research (Horizon 2020 COBRA) to develop a Co-free Li-rich layered oxide with stoichiometry $Li_{1.1}Ni_{0.35}Mn_{0.55}O_2$. This material has a high specific capacity (160 mAh g⁻¹ at 0.33 C and 100 mAh g⁻¹ at 1 C) and cycle life (80% capacity retention after 150 cycles at 0.33 C) at an affordable cost. We also explored a solution-based approach to improve the rate performance of NMC622 particles by coating them with a TiO_x shell. The application of the conductive shell increased the discharge capacity from 100 to 111 mAh g⁻¹ at 5 C.²

Creative chemical procedures were also used to synthesize a stable negative electrode material for sodium-ion batteries (SIBs). A carbothermal reduction reaction was utilized to form $Na_{2+x}Ti_4O_9/C$, a phase that can typically only be produced through a complicated synthesis process.³ The material has a discharge capacity of 124 mAh g⁻¹ and a capacity retention of 89% after 250 cycles at 1 C.

The IMO-Imomec group has developed a class of nonflammable liquid electrolytes for SIBs to enhance their safety. Through a combination of experimental and computational studies, the coordination structure of a deep eutectic solvent (DES) consisting of a sodium salt dissolved in *N*-methyl acetamide was optimized, offering a more durable electrochemical performance in full cells (97.0% capacity retention after 250 cycles at 0.2 C and 55 °C) as compared to conventional electrolytes.⁴ DESs were incorporated into inorganic and polymeric backbone structures, resulting in a new solid electrolyte class called eutectogel.^{5,6} The eutectogels had ionic conductivity values up to 1.46 mS cm⁻¹ and could be compatible with high-energy positive electrode materials such as NMC622, depending on their exact composition. The introduction of organic modification enhanced the mechanical properties of silica-based ionogels and ultimately improved the electrode/electrolyte contact.

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Operando Nuclear Magnetic Resonance study of the lithium plating mechanism for the optimization of Li-ion battery fast charge

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Li-ion batteries (LIBs) are now ubiquitous in our daily lives and are of first importance for our society, with applications ranging from small electronic devices to electric vehicles, but their limited lifetime still presents a great challenge for the generalization of transport electrification. They must be able to accept fast charges, even at low temperatures. However, during charge process at these conditions, formation of metallic lithium on the surface of the negative electrode made of graphite can occur and accelerate the capacity loss of the battery and thus the autonomy of the vehicle. In addition, if lithium metal deposition grows in the form of dendrites, the separator can be perforated, leading to internal short circuit in the battery. This degrading mechanism known as Lithium- plating is a key research axis to extend the life of batteries.

Therefore, a more global understanding, in real time, of this phenomenon and its kinetics in function of the local conditions within the negative electrode in a functional LIB is needed. In order to develop this understanding, it is crucial to perform operando analytical measurements on a working battery that allow monitoring different states-of-charge (SOC) repeatedly, in principle throughout their life cycle, giving access to a multitude of analytical data compared to a single ex-situ or post mortem analysis. In our study, we perform measurements by ⁷Li operando Nuclear Magnetic Resonance (NMR) on practical configuration: LiNi_{0.8}Mn_{0.1}Co_{0.1}O₂ (NMC811)/graphite pouch cells made with industry-grade electrodes and under realistic cycling conditions. This non-invasive and non-destructive technique is sensitive to both structure and dynamics. The ⁷Li NMR signal of Li ions in graphite electrode was recorded during electrochemical cycling over a wide range of current rates. This allows analyzing intercalation processes in the electrode, changes of Li-ion mobility, and Li metal deposition on graphite at high current rate due to an inhomogeneous distribution of ions induced by limitation of diffusion on solid and liquid phases. In our experiments, with a CC charge and a subsequent CV period at 4.2V, Li deposition starts at around 3.5 V well before the full lithiation of graphite and reaches a maximum of intensity during the voltage floating. During this phase, and due to the drop of the current, the lithium plating starts to interact with its environment by intercalating in the graphite structure or reoxidizing during the following discharge to transform into cyclable lithium. These different contributions will be more detailed on the presentation.

This work is funded by the FOCUS Battery project of the CEA.



Figure 1. Voltage profile and contour plots of operando ⁷Li NMR data recorded on a NMC811/graphite cell during galvanostatic cycling between 4.2 and 2.5 V at 0 °C









Spectroelectrochemical capabilities at the HIPPIE beamline: a new platform for operando characterization of battery interfaces

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HIPPIE is a high-flux, high-resolution soft x-ray beamline at MAX IV Laboratory (Sweden) with a new dedicated branch for operando studies of electrochemical interfaces. Such experiments utilize the dip and pull method to form a thin liquid meniscus on the surface of the working electrode. The solid/liquid interface can then be probed using photoelectron spectroscopy, whilst maintaining electrochemical control, making it ideal for probing oxidation state changes, chemical shifts, electronic structure and electrochemical potentials in-situ.

The new branch of the HIPPIE beamline operates in the 250-2500 eV range, providing access to the L absorption edges of many transition metals relevant to current and next generation batteries (e.g. Co, Fe, Zn etc). The endstation uses a state-of-the art ambient-pressure hemispherical electron analyzer for photoelectron spectroscopy (PES) measurements in vapor pressures up to 25 mbar. This allows operando PES measurements of a three electrode electrochemical cell with liquid electrolyte. An argon/nitrogen atmosphere glove box can be attached to the measurement chamber such that air sensitive materials can be studied. The system is compatible with common battery electrolyte solvents and many electrode materials (typically foils or thin films).

The objective of this new branch is to allow users to access the all-important chemistry that occurs at solid-electrolyte interfaces, which is of huge relevance to battery research. This poster will present the technical capabilities of the HIPPIE beamline that makes this possible, highlighting specifically how it can benefit the battery community.



Figure 1. Photograph showing the entrance cone of the hemispherical electron analyzer and a 3-electrode electrochemical cell.













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INSTABAT is a European project that forms part of the battery 2030+ initiative and its objective is to enable real-time monitoring of critical parameters within lithium-ion battery (LiB) cells from the development of physical and virtual sensors. In this way, **INSTABAT** aims to provide precise information on the cell's state of charge, health, power, energy, and safety to enhance the reliability and extend the lifespan of LiBs [1].

In this work a brief summary of the results regarding the physical optical fiber sensors developed in the frame of *INSTABAT* to physical monitor temperature and strain variations, and virtually temperature and state of charge (SOC) though thermal algorithms are presented. To strain and temperature monitorization, two studies were developed. One including a hybrid sensor composed by a fiber loop mirror and a polarization maintaining fiber Bragg grating (PM-FBG) for simultaneously measure temperature and strain variation on a surface of an 18650 LiB [2], and the other approached the strain and temperature decouple using the matrixial method applied to the different sensitivities of fast and slow Bragg reflections in PM-FBG sensors [3]. Regarding the virtual sensor developed, a work approached the development of a particle filter (PF) to predict the internal temperature and the SOC, using simulation data to feed the filter [4].

The data collected from these sensors would be analyzed in conjunction with physico-chemical degradation phenomena to identify potential areas of concern. The information thus obtained would then be integrated into enhanced battery management system algorithms to improve the performance and reliability of LiBs [1].





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Since 2019, and accordingly with the European Green Deal, several initiatives aim to transform the European Union economy toward a more sustainable future by reducing the emission of greenhouse gases (CO₂) and to improve the energy transition by mitigating climate change [1]. BATTERY 2030+ research initiative aims to contribute to carbon neutrality in the European Union by developing more sustainable batteries for the future, reducing the actual society's dependence on fossil fuel energy. *INSTABAT* project is a member of this initiative and aims to research smart batteries and develop new methodologies to sense critical parameters within the battery cells. However, as the batteries basically operate through extremely exothermic electrochemical events, special attention must be paid to their thermal, volumetric and gas evolution constraints, where continuous and accurate monitoring is of great importance for their quality, reliability, life extension, and safety operation [2].

Considering it, in the scope of **INSTABAT**, customized optical fiber sensors (OFS), based on fiber Bragg gratings recorded in standard and birefringent fibers, and hybrid sensors based on Fabry-Perot interferometers are being developed and instrumented into Li-ion batteries to simultaneously monitor internal and external safety parameters, such as temperature, strain, and pressure, during galvanostatic cycles **[3-5]**. As this sensing technology is immune to electromagnetic interference, reduced dimensions (125 μ m or less), and also present multipoint and multiparameter characteristics (a network of several OFS in one fiber line can be produced), they seem to be very promising tool to proceed with measurements of critical safety parameters in batteries, allowing their real time monitorization. From the results reported, good feasibility and reproducibility were observed in the developed optical sensor's performance and demonstrated that by operating as a multiparameter decouple system, they can decrease the complexity and intrusiveness in batteries and simultaneously monitor different parameters. In this way, the sensing data recorded can be a precise tool to 1) be used and correlated to internal electrochemical events and with the different battery states (SOX); 2) be integrated in machine learning algorithms for the virtual sensor's development; 3) extend the battery quality, reliability and life (Figure 1).



Figure 1. Customized physical OFS to monitor internal and external safety parameters in LiBs. The data form the sensed parameters can be a useful tool to used and correlated to internal electrochemical events and with the different SOX, to develop ML algorithms for virtual sensing, and QRL cell improvement.

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BATTERY 2030+ Annual Conference 2023

REFERENCE ELECTRODE AS NEW BMS SENSOR

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As some degradation mechanisms at electrode scale are initiated above or below a threshold in potential, implementation of a reference electrode within the lithium-ion cells could help to manage more precisely the charge/discharge cycles and gain in lifetime. As an example, lithium metal deposition contributes strongly to the capacity decay of the cell under certain charging conditions (fast current, low temperature)¹. Its formation is made possible because of an overpotential effect on the negative electrode profile that is lowered towards values close or below to 0V vs. Li*/Li. Likewise, electrolyte or crystal of NMC can degrade at high potential and high temperature^{1,2}. That implies that the reference electrode is capable of providing a reliable and stable response over time. FePO₄/LiFePO₄ (LFP) is the reference electrochemical couple chosen because it presents a potential plateau over a wide range of lithiation. The presentation will give, in a first part, an evaluation of the duration of stability in potential of the reference electrode. In a second part, we will report the profiles in potential of monolayer NMC622/graphite pouch cells under cycling (according to a standard vehicle profile formulated as a worldwide harmonized light vehicle test cycle (WLTC)³ for discharge and charge 1C) and at 4 different temperatures. The excursion in some ranges of potential where lithium-plating formation is possible or electrolyte/cathode degradation occurs can be thus known. A correlation with post-mortem analyses will give answer about the consistency of the response in potential given by the reference electrode and for example if it is able to detect the formation of localized metallic lithium.





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Enhancing the Performance of Na₂FeP₂O₇ and Na_{0.67}MnO₂ Cathodes for Sodium-Ion Batteries

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Sodium ion batteries (SIBs) are considered an alternative for stationary energy storage due to the high abundance of sodium content and relative similarity to lithium-ion batteries (LIB). However, SIBs face challenges including relatively low energy density compared to LIB. In this work, we explore ways to improve the electrochemical properties of the SIB cathode materials Na2FeP2O7 and Na0.67MnO2.

Na₂FeP₂O₇ is a promising cathode material for SIBs but has low electrical conductivity – approximately 10-7 S/cm when extrapolated to room temperature according to our measurements [1]. We prepared Na2FeP2O7/C composite, optimized carbon content and found that the addition of carbon increases the capacity up to 92 mAh/g, with excellent rate capability and no capacity loss over first 500 cycles in FEC-containing 1 M NaClO4 in PC electrolyte [2]. The obtained results are largely due to smaller grain size and improved conductivity. We also found that addition of reduced graphene oxide (rGO) does not improve electrode kinetics, with the effect being proportional to the amount of rGO.

Layered P2-type oxides are another material class widely studied cathode materials for SIBs. We prepared Na_{0.67}MnO₂ and found that its performance is extremely dependent on the binder used [3]. Sodium alginate binder is able to significantly improve the cycle life while a novel tetrabutylammonium (TBA) alginate binder show 6 % increased gravimetric capacity values and improved rate capability.

Overall, our study not only investigated the preparation of two materials for Na-ion batteries, but also shows that the choice of binder, electrolyte and electron-conducting additives can significantly improve the electrochemical properties of electrode materials for SIBs. These aspects must be considered in the development and testing of other electrode materials for SIBs when developing sustainable and long-lasting energy storage solutions.

The financial support of projects No. 1.1.1.2/VIAA/1/16/166 "Advanced materials for sodium Ion batteries" and No. lzp-2020/1-0391 "Advanced polymer – ionic liquid composites for sodium-ion polymer batteries" is greatly acknowledged. Institute of Solid-State Physics, University of Latvia as the Center of Excellence has received funding from the European Union's Horizon 2020 Framework Program H2020-WIDESPREAD-01-2016-2017-Teaming Phase 2 under grant agreement No. 739508, project CAMART2.

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Polyanion Insertion Material as a Catalyst for Oxygen Electrocatalysis

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Electrocatalyst-based energy-storage technologies such as alkali-metal-air batteries, fuel cells, water splitting devices are the new holy grail for the next-generation energy storage landscape as they deliver high energy densities than lithium-ion batteries (LIBs), it also mitigates the dependency on traditional cathode materials used in LIBs and has more diverse catalyst-based cathodes. Practically, perovskite oxide-based electrodes are the most active and widely studied catalysts to perform oxygen electrocatalysis (ORR and OER) reactions. O₂ electrocatalysis exhibited by transition metal phosphate-based (PO₄)³⁻ polyanionic material has also dented its place and showed superior performance, shown potential application as a cathode in a metal-air battery application.¹ Despite of the respectable current densities and promising overpotentials delivered by these (PO₄)³⁻ based catalysts, these materials suffer from poor stability in highly alkaline aqueous based electrolyte. Thus, phosphate-based polyanionic battery material will be discussed with different kinds of transition metal as catalysts, addressing the influence of coordination of oxygen around the metal, phosphate units and alkali cation.² The underlying mechanism explaining the active site in phosphate-based catalyst will also be highlighted.

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CONTROL-ORIENTED THERMAL MODELING OF BATTERY CELLS FOR OPTIMAL TAB AND SURFACE COOLING

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Tab cooling offers homogenous cooling of the electrode stack leading to a significant reduction in temperature gradients, thus prolonging battery lifetime. However, surface cooling is more effective at removing heat due to the larger surface area of batteries, leading to a lower average temperature. This trade-off between the ability of a cooling method to maintain a low cell average temperature and that to minimize thermal gradients within the cell necessitates the need to combine these two cooling methods to optimize their individual strengths. In this study, we present a 2D battery thermal model that allows independent control signals for the tab and surface cooling channels making it ideal for optimizing thermal performance by effectively manipulating the channels. The model is based on the Chebyshev Spectral-Galerkin (CSG) method and has the potential to predict the spatially resolved full temperature distribution throughout the cell with a similar computational efficiency to that of thermal equivalent circuits. We validated the model for a typical large format cylindrical lithium-ion battery through comparison with a high-fidelity CSG model with 100 states under pulse heat generation profiles and the Worldwide Harmonised Light Vehicle Test (WLTP) drive cycle. The results showed that the developed model with only 2 states can capture the 2D temperature field, and that in highly transient thermal applications, a model order of 9 states can improve accuracy significantly. The model has the potential to be seamlessly integrated with an electrical, degradation and mechanical model to investigate various cases of interest such as ageing phenomena and internal short circuits. In addition, it can be used to mimic and investigate state-of-the art such as immersion and all-tab cooling. Furthermore, this study sets the stage for an optimal cooling scheme selection that will inform battery manufacturers on optimal sizing for optimum thermal performance.

Keywords: Battery thermal management, Control-oriented low-order modeling, Thermal model, Spectral-Galerkin method, Lithium-ion battery, Electric vehicle

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NSTABAT sensibat



SMART BMS Testing for advanced SoX estimation

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The Li-ion (Lithium-ion) battery technology is crucial for electromobility because it offers several advantages over other types of batteries. Firstly, Li-ion batteries have a high energy density, which means they can store more energy per unit volume or weight than other battery chemistries. This is important for electric vehicles because they require high energy to power the vehicle over long distances. Secondly, Li-ion batteries have a high power density, which means they can deliver a lot of power in a short amount of time. This is important for electric vehicles because they need to be able to accelerate quickly and respond to sudden changes in driving conditions. Thirdly, Li-ion batteries have a long cycle life, which will help to build more desirable business models. This is important feature for electric vehicles because they need to be reliable and have a long lifespan.

However, this lifespan could not be necessary for some application such as specific electric vehicle applications, heavy duty applications where longer cycle life is expected due to higher usage, stationary and some other applications. In this sense, SPARTACUS project is focused on the development of new sensors for evaluating cell temperature map, cell swelling process by using pressure sensors and ultrasound wave properties such as time of flight or young modulus. Then, this data will feed advanced SoX algorithms to monitor inner cell state with higher accuracy than conventional BMS approach. The final objective of this work is to evaluate the increase of lifetime generated by new BMS functionalities compared to conventional BMS. Conventional BMS aging test are already conducted, and it is planned to start the aging tests as soon as possible.

At this stage of the project, CIDETEC was able to build Hardware in the loop system to be able to run a virtual BMS (conventional and SPARTACUS BMS) and to conduct aging tests, evaluating the capacity fade and impedance rise periodically. In this virtual BMS, a conventional BMS logic was implemented and the goal is to implement SPARTACUS smart BMS to rung aging. However, during this period it was possible to evaluate some smart BMS functionalities, such as temperature and pressure sensors, as it is visualized in the next figure. Two different layers were built and stacked with the cell, measuring 6 temperature and 4 pressure sensors.



Figure 1. Smart BMS test set up with some preliminary temperature and rubber sensor results.

In the publication, obtained preliminary results on advances Lithium-ion sensing will be detailed. Additionally, more details of the developed Hardware in the loop system will be provided, which enables the measurement of different variables, running of different BMS strategies and controlling of cell testing device automatically ensuring safe use of batteries, by supervising all the data provided by each sensors









Synthesis of glass-ceramic Li₂S-P₂S₅ based electrolyte for solid-state batteries

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Solid-state electrolytes for batteries have been of interest in recent years because of their increased safety over their liquid counterpart that suffer from problems such as leakage, ignition, and explosive risks. [1] Currently solid-state electrolytes suffer from problems like lower ionic conductivity and worse contact with electrodes compared to liquid electrolytes. These are all problems that need to be solved to successfully replace liquid electrolytes. [2] One promising type of solid-state electrolyte is based around the Li₂S–P₂S₅ binary system. Glass ceramic electrolytes based on this system are interesting because of their high ionic conductivity and non-flammability. An interesting composition in this system is the 75Ll₂S-25P₂S₅ composition which have been known to reach relatively high ionic conductivity (above 10^{-4} Scm⁻¹) after heat treating. This increase in ionic conductivity is thought to be related to the formation of crystalline β -Li₃PS₄. [3] These electrolytes are normally synthesised using melt quenching but can also be synthesised more easily using a chemomechanical technique such as ball milling. [4] Couple of issues exist currently with Li₂S-P₂S₅ electrolytes one is their poor air stability since the electrolyte easily reacts with moisture in the air to form H₂S [5], meaning that every preparation step needs to be performed in an inert atmosphere leading to many extra steps during production. A problem that also need to be solved is the incompatibility with the electrodes.

The aim for this project is to synthesise a solid-state glass ceramic $Li_2S-P_2S_5$ based electrolyte using the ball milling method. An amorphous glassy material is formed using ball milling and turned into a glass ceramic with subsequent heat treating to facilitate crystal growth. The system is doped with Li_4SiO_4 resulting in a chemical composition of $75Li_2S$ (25-X) P_2S_5-XM where X is the mole percentage of the dopant and M is the dopant. Goals for the electrolyte is to have high ionic conductivity and compatibility with electrodes which we investigate using methods such as Raman spectroscopy, electrochemical impedance spectroscopy (EIS) and X-ray photoelectron spectroscopy (XPS). These results will be important for the application of this electrolyte in all-solid-state lithium batteries.

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The need to reduce the carbon footprint is growing rapidly. Green energy systems such as wind, solar, tidal and others are constantly being integrated into our electricity grids to limit fossil fuels use in energy generation. With the green course implementation, new challenges arise such as the need for energy storage during the period when energy production is most active but consumption is the lowest. Battery technology, as one of many energy storage technologies, is receiving a lot of attention for energy storage [1]. Since Zn-MnO₂ battery technology is one of the oldest known battery technologies and has one of the highest potential for use in large-scale energy storage systems, it has received increased attention from researchers [2-3]. In this work, we show an interesting approach to designing a Zn-MnO₂ battery, which involves creating a battery from two different electrolytes. The electrolytes are prepared in such a way that they improve the performance of each electrode, i.e. the basic electrolyte is used on the anode side and the acidic one on the cathode side. Applying this approach allows to increase the battery potential to 2.4V.

The developed amphoteric battery (Fig. 1.) consisted of Zn foil as an anode, $MnO_2/carbon$ black mixture as a cathode, and Pluronic F-127 acidic (H₂SO₄) and basic (KOH) hydrogel as electrolytes. No membranes were used in the battery construction. The use of this unique dual electrolyte increased the open circuit potential of the battery and prevented the formation of an insoluble ZnMn₂O₄ compound, allowing the battery to be repeatedly charged and discharged.

As a result, a membrane-free rechargeable amphoteric Zn-MnO₂ battery with an open circuit potential (OCP) of 2.4 V was obtained. The OCP of the formed battery was stable for more than 25 hours, after which the pH and electrical conductivity of the two electrolyte environments changed due to the mixing of the acidic and alkaline hydrogels. This change is very clearly reflected in the battery impedance measurement (measuring battery parameters every hour), where a rapid increase in internal resistance can be observed from 25 to 30 hours. During this time, active acid and alkali neutralisation occur, resulting in a decrease in the number of ions in the electrolyte and the formation of an electrically neutral water molecule. This indicates that additional research is needed in the development of hydrogel electrolytes. Also, 200 charge-discharge cycles were performed while maintaining a stable OCP. About 2.3 V OCP was maintained before cycling, after 100 and 200 cycles.



Figure 1. Operation and scheme of the created amphoteric battery.

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Integrable Multi Sensor Array for Improved Aging Detection in Lithium-Ion Battery Cells

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Today, Lithium-ion batteries are the most used energy storage technology in many applications. So, there is strong incentive to further improve its sustainability. Improving diagnostics, in particular the measurement and prediction of the remaining capacity can lead to a longer lifetime and safer use, thereby saving energy by keeping resources in circulation for a longer period.

One approach to improve diagnostics is the monitoring of the mechanical properties of LIBs to detect degradation before it effects performance and capacity. In particular chemical side reactions within the cell lead to the formation of by-products (e.g. solid electrolyte interphase (SEI), plating). These degradation products change the mechanical properties of the LIB (e.g. thickness, sound velocity that is dependent on the Young's Modulus). Therefore, measuring cell thickness and sound velocity via dilatometry and ultrasound (US) can provide valuable insight into the current and projected state of health of a LIB cell. In a laboratory environment dilatometry and US measurements show promising results and correlate well with battery deterioration ^[1].

In this work, we address the challenge of how to detect these mechanical changes within a LIB in a cheap, packintegrable way with local resolution setup. For this purpose, five piezo electric transducers are mounted in pairs on opposing sides of a LIB cell onto a specially designed flexible printed circuit board (PCB). With these pairs of piezo transduces, the time of flight of the ultrasonic wave through the cell can be measured on five different locations. Beside the ToF, the Fourier transformed power spectra can be also evaluated. To measure the dilation/pressure a dielectric elastomer sensor (DES) system was developed specifically for the monitoring of the expansion of the LIBs. This thin and soft compression load sensor can also serve as a compression pad and absorb irreversible thickness gain of the cells without leading to an unhealthy increase of pressure. Eight of these Sensors were spread over the area of the cell. Furthermore seven temperature sensors were placed directly in contact with the pouch on the PCB. These can detect unhealthy operating conditions and correct the other measurements for temperature variations.

The layout of the sensor mats and an exemplary measurement of four dielectric elastomer sensors is shown in Figure 1. The data shows that the thickness changes during a C/10 cycle can be measured. Significant thickness changes were measured at the expected phase transitions of the active material ^[1].



Figure 1. Dilation over Capacity and differential Dilation dx/dV over Voltage for 4 sensors (left). Schematic (middle) and images (right) of the sensor array.

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BAT4EVER

HIDDEN INSTABAT sensibat





Integration of printed graphene-based reference electrodes in lithium-ion batteries for advanced battery management systems

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In order to improve the lifetime and safety of lithium-ion batteries (LIBs) by eliminating the LIB degradation phenomena (e.g. cathode overcharging, abnormally anode potential increase during over-discharge, and side reactions during the over-discharge), collecting accurate data during LIB operation is required. The electrochemical behaviour of LIB components could be studied by electrochemical measurements using threeelectrode LIB cells, which can focus on the behaviour of each individual electrode. The reference electrode could monitor independently the anode and cathode potential (thanks to their ideally constant equilibrium potential) and thus the impedance contributions can be evaluated. Using conventional LIB reference electrodes such as point-like, ring-like, and coaxial reference electrodes cause geometric and electrochemical asymmetries, which this phenomenon eventually leads to electrochemical impedance spectroscopy (EIS) measurement artifacts [1]. The proper location, shape, and morphology of the electrodes minimize or fully avoid common EIS measurement artifacts. The geometric/electrochemical asymmetries effects could considerably decrease in mesh-like reference electrodes. In the ideal mesh-like reference electrodes with a thin and large opening ratio (to minimize Li-ion blocking effects), the ions can travel in the electrolyte through the openings of the mesh. In this study, the novel printed reference electrodes based on lithium salts, namely lithium titanate and lithium iron phosphate, and single-/few-layer graphene flakes were produced using the screen printing deposition technique for accurate monitoring of cathode and anode potential (e.g., control of Li plating at the anode and electrolyte decomposition at the cathode in presence of overcharging) as well as electrical modelling. The flat nature of the reference electrode printed on the battery separator (Celgard 2500) compared to conventional reference electrodes eliminates excessive compression stresses on the cell components [2]. The influences of the conductive materials and binder content on the electrode resistance and electrochemical performance are evaluated to find the optimal electrode composition. The obtained results confirm that the produced printed reference electrode can effectively monitor the potential of both anode and cathode with satisfactory reproducibility over cycling at C/5 C-rate. Thanks to the electrical and mechanical properties of graphene flake, its incorporation into the reference electrode formulation permits obtaining the desired electrical conductivity of the reference electrodes and ensures long-term stability (over 400h) of the reference electrode potentials because of the superior mechanical robustness of the reference electrodes provided by graphene [3]. The impedance contribution of the reference electrodes was properly modelled through a mesh-like electrical equivalent circuit and obtained results showed that the characteristic frequency of the produced printed reference electrodes is higher than 100 (kHz), which is satisfactory to carry out valuable EIS measurements of the LIB electrodes. The electrochemical properties of twoand three-electrode pouch cells were comparable, confirming that the insertion of the printed reference electrode in the cell does not significantly alter the performance of the full cell.

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EFFECTIVE SCIENTIFIC DATA SHARING WITHIN BATTERY2030+

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BIG-MAP aims at accelerating the discovery of battery materials and interfaces. This is accomplished via the development of a shared data infrastructure capable of autonomous acquisition, handling, and analysis of data for the entire battery development cycle. At the heart of this platform lies a private data repository named BIG-MAP Archive¹, which enables humans and machines from BIG-MAP to store and exchange curated scientific datasets and their associated metadata. After a presentation of the repository and its capabilities, we will discuss (1) the possibility to open it to the whole BATTERY2030+ community and (2) the possibility for users to easily copy their stored datasets to the open-access repository Materials Cloud Archive, where they will receive persistent DOIs and a guaranteed lifetime of at least ten years from submission.





Figure 1. The homepage of BIG-MAP Archive.

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Nucleation pulses to control dendritic growth in sodium-metal batteries

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Electrification in all sectors, as an indispensable alternative for sustainable development, has led to an unprecedented demand for energy storage devices. Although current generation of lithium-ion batteries has desirable performance and reliability, limited resources of the elements such as Li, Ni, and Co affect their availability on a long run. Sodium-ion batteries (SIBs) on the other hand can be a good option due to the abundance of Na element and similarities between Li and Na elements. Since cathode material for SIBs has reached a stage of commercial production, the search for a high energy density anode material is the main challenge to overcome. Sodium metal can be the material of choice as soon as the dendritic growth during electrodeposition is prevented.

In this work, electrochemical strategies are used to induce two-dimensional growth and minimize dendrite formation during electrodeposition of sodium. High overpotential pulses are applied before oxidation (stripping) and/or reduction (plating) steps and the effect of these nucleation pulses is studied by means of chronopotentiometry. Symmetrical three-electrode cells with sodium as working, counter, and reference electrode are used in electrochemical measurements. Additionally, ex-situ SEM imaging is used to relate the resulting morphology of working electrodes to the chronopotentiometry profiles.

Initial results show the positive influence of various nucleation pulses on inhibiting formation of the dendrites. The results prove that electrochemical strategies can be used as a beneficial tool to control dendritic growth and encourages for further investigation on different electrolyte compositions to help with the issue.












e-TROVA Diesel-to-Electric technology

Joris de Hoog¹, Nick de Bie² ¹ Flanders Make ² Flanders Make ³ Third Affiliation

e-TROVA's vision is to enable the realization of the emission reduction targets for transport as set forward by the Green Deal. This Flemish company is founded in 2021, in alliance with the US based Trova CV. e-TROVA offers diesel-to-electric repowering of heavy-duty trucks with a range up to 300 km. The retrofit conversion will be done in 48 hours for multibrand N3 class trucks. This includes different brands, types and years of manufacturing.

Flanders Make is the subcontractor for e-TROVA for all engineering activities. This includes the design and architecture of the electric powertrain, reverse engineering, the selection of the VCU (Vehicle Control Unit) and the development of the vehicle software. With respect to the high-voltage battery, different topics are covered namely sizing, vehicle integration, testing & validation and research towards upcoming technologies. Regarding sizing, Flanders Make defines the driving and charging performance targets. These are simulated using a simulation environment developed by Flanders Make. This environment is also able to simulate the lifetime of the battery given a realistic driving profile. With respect to integration, the mechanical and electrical integration are covered together with the software integration (BMS communication, cooling and charging strategy etc.). The testing & validation consists of validating the performance targets. This can be done by either using the Flanders Make battery testing infrastructure including a climate chamber (-60...130 °C), chiller and electrical source/sink (1000 V – 200 kW, 1500 V – 540 kW in Q3 2023). Another possibility is by real driving. The research activities focus among others on cell chemistries, battery pack cooling concepts and cloud environments.









INSTA**BAT** sensibat



Hybrid battery energy storage system for full-electric marine applications

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The International Maritime Organization (IMO) predicts between 50% to 250% increase in CO2 emissions from shipping industry by 2050 [1]. The full battery-electric propulsion system is a promising solution to move towards zero-emission marine transportation. The current traction batteries in the marine industry are based on the single type of battery, either high-energy (HE) or high-power (HP). Utilizing a monotype battery topology to comply with the vessel's requirements results in a battery system oversized either in energy or power. This study investigates the optimal sizing and cost assessment of the battery hybrid energy storage system (HESS) by integration of HE and HP Li-ion cells for a harbor tug [2], considering the required design life of the battery in marine sector. This is achieved by the development of novel battery system with separate power converters for each type of module and the development of a novel, highly dynamic and fast switching energy management system (EMS), that is capable of drawing power from the most optimal source depending on the operating conditions and operational requirements, while also optimizing battery lifetime. A battery pack with a guaranteed lifespan of 10 years while cycling in the SOC range between 90% and 10% will be developed in the context of this project. Finally, a cost-benefit analysis is performed showing a clear topology that is optimized for both power, energy and cost. The system will be built and demonstrated in a Damen Electric Tug 2513, as shown in Figure 1.



Figure 1. Damen electric tug 2513

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Real time estimation of electrochemical states in Li-ion batteries and exploitation in BMS algorithms

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In order to enable the development of advanced Battery Management System (BMS) algorithms, having realtime access to spatially-resolved values of electrochemical variables inside the battery cell is a promising avenue of research [1]. Accurate electrochemical models have been developed for simulating these systems, such as [2] systems, yet these models are not suited by themselves for real-time monitoring of the battery states since they usually have a high computational cost and require a good knowledge of the initial state of the system and the system parameters. Some examples of models used in this context are [3,4]

State estimators based on electrochemical models, such as [5], simultaneously leverage existing knowledge of the system (in the form of reduced-order electrochemical models) and the robustness properties of feedback systems. By monitoring the values of some measured variables (such as current, terminal voltage and reference electrode voltages) in real time, these algorithms adapt their state estimations. The use of measurement values has the advantage of increasing the prediction performance of models, allowing for a lesser computation complexity for equivalent prediction performance (thus allowing the algorithms to run in real time).

In the context of the INSTABAT project, we present an improved version of an electrochemical observer, based on the work done in **[5]** and integrating heterogeneity in the lithiation process in the electrodes and present some ideas on how this can be exploited by new BMS SOX indicators. Beyond improved SOC estimation, the physics-based model is integrated inside an estimation algorithm of the power capability of the battery cell aiming at preventing the battery from moving outside its safe operating area. The estimation of the maximum available power is achieved by formulating and solving a constrained nonlinear optimization problem.

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Probing the Solvation Structures of Battery Electrolytes through NMR Spectroscopy

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The microstructure of electrolytes is known to regulate physicochemical properties such as ionic conductivity and redox stability **[1]**. Numerous electrolytes have been introduced to improve the performance of batteries, including lithium salts, solvents, and additives. However, the detailed Li⁺ solvation structure in the organic electrolytes is not fully known, which represents a bottleneck for developing better electrolytes. Herein, we present our study to probe the solvation structure of battery electrolytes through NMR spectroscopy. We successfully evaluated different solvation structures and compared them to experimental data, demonstrating agreement between the calculated average of ⁷Li NMR chemical shifts of highly populated structures **[3]** and experimental values **[3]**. This work has significantly implications for the development of new battery electrolytes for more efficient and sustainable energy storage systems.

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INSTABAT sensibat



Self-Healing Binders for Silicon-Based Electrodes

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Silicon is a promising active material for anodes in lithium-ion batteries owing to its high theoretical capacity (3579 mAh/g) [1]. However, it is well known that the compound contends with large volume changes during cycling, creating cracks in the material and therefore limiting the lifetime and capacity of the cell. To cope with these volume changes, this project aims to develop self-healing binders to improve the cycling stability of lithium-ion batteries.

Both hydrogen bonds and dynamic covalent bonds have previously been used to modify binder systems to get self-healing properties through reversible cross-linking with the binder in the electrode. While the hydrogen bonds have eminent reversibility, the dynamic covalent bonds provide higher mechanical stability [2-4]. Both of which are desirable properties to implement in the polymeric binder system.

Specifically, the focus of this work has been to use borate ester bonds [5] and couple them with the polymeric binder poly(vinyl alcohol). Furthermore, in order to gain more knowledge of the different self-heling groups and how they anchor to the binder, other binder systems containing carboxymethyl cellulose have been used for comparison.

The electrochemical performance of the cells with and without the self-healing groups has been investigated, showing an increased capacity with the latter. Besides the performance, the morphology of the cells is shown through Scanning Electron Microscopy where the electrodes with the modified binder show less cracking both previous to and after cycling. Furthermore, the electrochemical stability of the functional groups was investigated to compare the impact of the dynamic covalent bonds, especially at the low operating voltages of silicon.

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Aerofit Batteries – Integrated cell to system development for climate-neutral aviation

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Abstract CO₂ emissions are the main driver of global climate change with aviation accounting in 2020 for 2.5% of global CO₂ emissions (and 3.5% of global warming potential) [1,2]. Electrification of aircraft propulsion is considered as one key enabler for tackling the challenge of reducing greenhouse gas emissions from aviation.

Battery technologies fit for upcoming fully- and hybrid- electric aircraft from commuter to regional (50+ pax) size as well as their system integration face various challenges:

- Specific cell designs considering the particular requirements of aeronautic applications, optimizing potentially conflicting targets between energy power cyclability safety;
- Lightweight, safe and scalable (up to MWh-class) battery packs with integrated sensing/monitoring, and electrical and thermal management;

Adequate numerical tools for performance, ageing and safety modelling capable of bridging cell to large-scale system integration taking into account aeronautic certification standards are required.

Within several EU funded research projects (HE HighSpin, HE HELENA, H2020 IMOTHEP, H2020 ORCHESTRA, CA HECATE), AIT pushes the development of next generation electrochemistries, aeronautic cells and modules and aspects of aircraft system integration as well as the integration of electrical energy storage into aeronautical structures (CS2 SOLIFY and HE MATISSE). The AIT HEAT research team pursues an integrated model-based cell-to-systems approach taking advantage of the outcome of in-house battery development and testing to accelerate aircraft electrification.

A large amount of data generated in these projects at various levels from material and cell characterisation, manufacturing to performance and safety testing, and simulation needs to be handled in a structured way to make them FAIR (Findable, Accessible, Interoperable, and Reusable). To address this challenge within AIT, we aim at building up a battery database upon the BattInfo ontology developed in BIG-MAP.

This poster presents the integrated AIT approach and the data management under development.



Figure 1. Aerofit battery challenges and AIT approach.

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Automating XANES Simulation of Battery Materials with AiiDA

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X-Ray absorption spectra (XAS) has been an invaluable tool in the research of new battery materials[1] due to its capacity to probe the local chemical environments within a material and grant insight on the structural changes which occur during operation of the battery system. For Li-ion batteries (LIBs), such changes are notable in the case of the lithium nickel oxide (LNO) cathode material, which is known, both from experimental studies[2] and recent computational works[3], to adopt various crystalline phases during battery cycling. Furthermore, operando XAS studies of LNO[4] also demonstrate a consistent shift of the Ni K-edge to higher energy as Li moves from the cathode, which has been attributed to a gradual shift of the average Ni oxidation state from Ni(III) to Ni(IV). In this work, we demonstrate at the atomistic level the effect of changes in the oxidation state of Ni in LNO on the Ni K-edge as a function of Li content. Using reliable and accurate automated workflows within the AiiDA automation platform[5] to compute K-edge XAS spectra at the density functional theory (DFT) level, we compute fully-resolved XAS spectra for a range of crystalline phases of (de)lithiated LNO and demonstrate the site-specific contributions to the final K-edge spectrum - showing clearly the effect of the Ni oxidation state on the XAS spectrum at the atomistic level.



Figure 1. Simulated XANES Spectra for pristine and de-lithiated crystalline phases of Li_xNiO₂. Photon energies given relative to a Fermi level of 0eV

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SPARTACUS

HIDDEN Project

Self-healing thermotropic liquid crystalline electrolytes to enhance the lifetime and increase the energy density of Li Metal Batteries

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The HIDDEN project develops self-healing processes to enhance the lifetime and to increase the energy density of Li-metal batteries 50 % above the current level achievable with current Li-ion batteries. The HIDDEN consortium develops materials and their processes to functional battery layers as scalable, industry compatible, manufacturing technologies enabling sustainable energy storage technology with longer battery lifetime and higher energy storage capacity for more efficient utilization of sustainable, carbon free energy production technologies.

HIDDEN develop novel self-healing thermotropic liquid crystalline electrolytes investigate both technologies with protective additives, and apply multiscale modelling means for electrolyte design and analysis algorithm to monitor the dendrite growth. Technologies will be upscaled from laboratory to industrial manufacturing

The simplified schematic images in Figure 1 explain the basic principles of the selected self-healing methods (not in scale), i.e. (a) utilization of TILCs to break the formed dendrites mechanically during phase transitions and upon heating above their clearing point.



Thermotropic liquid crystalline electrolyte molecule

Thermotropic ionic liquid crystals (TILCs) **[1] [2] [3]** represent the "fusion" of two materials science concepts: the tuneable by design dynamically self-assembling (and therefore inherently self-healing) thermotropic liquid crystals (TLCs20), i.e. functional materials showing a thermodynamically stable but dynamic state of the matter with ionic transport ability of organic (liquid) and soft-matter-based (gel and polymer) electrolytes.

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Single Ion Monomers & Polymers Toward a high conductive and safer lithium battery electrolyte

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In 1996, M. Armand et al discovered the interest of perfluorinated amides salts (e.g. LiTFSI) and their uses as ionic conductive materials.

TFSI moiety is considered as the best candidate for Li salt in lithium batteries.

For 6 years, SPECIFIC POLYMERS proposed to the whole R&D Battery community methacrylic and styrenic-based monomers LiTFSI monomers namely MTFSILi (SP-49-023) and STFSILi (SP-59-011), as promising precursors to be used in electrolyte formulation or to prepare single-ion polymer electrolyte.



Figure 1. Chemical structure of Single Ion Monomers

It is noteworthy that polymerization of such salts can be performed by conventional or controlled radical polymerization (NMP, RAFT or ATRP).

These homopolymers are available in SP portfolio for 3 years under the references PMTFSILi (SP-4P-6-004) and PSTFSILi (SP-5P-9-009).



Figure 2. Chemical structure of Single Ion Polymers.

J. Gao et al.,[2] put forward that Single Ion Conductors has advantages over binary-ion conductors such as their high ionic selectivity against lithium approaching unity, their high oxidation voltage (>4.0V) as well as their resistance to dendrite formation. For instance, in a paper of J. L. Olmedo-Martínez et al [3] the PMTFSILi was mixed with different molecular weight of PEO. The impact of PMTFSILi on the crystallization and conductivity of the blends was explored in detail and it was proved that PMTFSLi has ability to reduce PEO crystallinity due to a great miscibility between both polymers. It has been demonstrated by L. Porcarelli and coworkers[4] a thermally-cured LiMTFSI/PEO-based single-ion conducting polymer gel electrolyte displaying simultaneously transference number (tLi+) ~1 and ion conductivity of ~10-4 S/cm at 25°C. More recently, Arrese-Igor et al [5] have demonstrated that PSTFSILi enhance the performance of cells (larger initial and most constant polarization).

HIDD

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Advancing understanding of battery materials through operando experiments using the 4th generation high energy X-ray source

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Complete physico-chemical operando characterization of electrochemical devices for energy conversion and storage is necessary to guide the development and to improve the performance. High brilliance synchrotron X-ray sources play a crucial role in this respect as they act as a probe with relatively high penetration power and low damage potential. ESRF underwent a major upgrade several years ago and provides even higher brilliance and, more importantly, coherence. This upgrade is particularly advantageous for beamlines providing high energy X-rays as they allow use of advanced scattering techniques with highly penetrating probe. Therefore, the techniques typically used for ex-situ measurements or at lower X-ray energies could be used on materials in half-cells and operating electrochemical devices. In this contribution the new possibilities of using high energy, high intensity, coherent X-rays to probe model systems and whole electrochemical devices will be presented.

To study batteries as a whole, elastic scattering techniques such as wide angle and small angle scattering are typically employed, as they can provide important complementary information to more standard X-ray imaging and tomography. The advantage is that the chemical contrast and sensitivity at atomic and nm scales is superior. Coupling these techniques with the tomographic reconstruction (XRD-CT and SAXS-CT) is much less common as it requires bright synchrotron sources, fast 2D detectors and advanced instrumentation [1]. However, such a combination allows spatial reconstruction of materials important atomic parameters in operando conditions. This will be demonstrated on imaging 18650 Li-ion battery during charge and discharge.



Figure 1. XRD-CT reconstructions of battery[2] (left). Phase transition in NMC cathode [3] (right)

Furthermore, local atomic and mesoscale structure, together with defect content, can also be determined by using Rietveld fitting, Pair Distribution Function (PDF) analysis and advanced SAXS theory. This in principle allows holistic investigations of composite materials at the battery level and understanding the interplay between different phases during operation. These are critical questions needed to be answered in order to incorporate novel materials into the electrochemical devices. Examples will be given on studies of the battery electrodes and electrolytes.

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SPARTACUS

From atomistic simulations of battery materials to a BIG-MAP*

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The performance of present generation Li-ion batteries may be sufficient for handheld devices, but it is still not sufficient to completely electrify the car fleet. This disruptive step requires a deep understanding of the materials in the battery cell down to the atomistic level. Both to increase the nominal charging capacity and to understand the aging processes. This can only be achieved by combining experiment and advanced simulations with data driven methods.

This poster presents how Dassault Systèmes (3DS) is participating in creating the Materials Acceleration Platform for the Battery Interface Genome(BIG-MAP). We start by investigating the processes leading to the formation of the Solid Electrolyte Interface (SEI) using a combination of Density Functional Theory (DFT), molecular dynamics(MD) and kinetic Monto Carlo(kMC). The combined kMC/MD method uses kMC steps to perform chemical reactions and MD to equilibrate the system between the reactions. The reaction rates were derived from DFT calculations of reaction barriers for the reaction steps using the FlexTS approach to molecules embedded in a COSMO implicit solvent. These MD/kMC simulations initially show the build up of organic reaction products, which are later pushed away from the anode surface as the inorganic layer is being formed [1].

To enable a comparison of this picture to experiment, spectroscopic finger prints were calculated by DFT. Theoretical XPS-spectra were calculated by DFT for atomic clusters that were cut-out from the atomistic structure models of the SEI layer derived from the MD/kMC simulations. The theoretical XPS-spectra show significant shifts depending on the local environment, which can be related to the spacial location of the target molecule with respect to the different layers of the SEI as indicated in Fig. 1 [2].





These types of simulations have been incorporated into an internationally distributed Materials Acceleration Platform (MAP) to optimize the electrolyte formulation with respect to density and viscosity. 3DS contributed the simulation tenant to deliver data for density and ion conductivity derived from MD simulations. Ecole Polytechnique Federale Lausanne (EPFL) provided a theoretical estimate of the ion conductivity. Karlsruhe Institute of Technology (KIT) delivered experimental data for density and viscosity. Danish Technical University (DTU) was running an adaptive Gaussian optimizer to optimize the electrolyte formulation with respect to density and viscosity. The communication between the tenants was controlled by the FINALES broker server. The test run proved that this distributed MAP was able run autonomously. The results from the test run showed a strong dependency of the ion conductivity on the LiPF6 concentration, but only limited variation of ion conductivity with respect to the solvent formulation[**3**].

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SPATIALLY RESOLVED RESISTANCE MEASUREMENT OF ELECTRODE SHEETS

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An important way to reduce Lithium-Ion battery cell cost is to reduce the production scrap rate, such that less of the expensive raw material is thrown away in faulty product. To achieve low scrap rates important characteristics of intermediate products, need to be checked along the manufacturing chain, and the information must be fed back to the process to take corrective actions. Currently manufacturers use various imaging technologies, such as X-ray radiography, X-ray tomography, ultrasonic scanning to, e.g., supervise electrode coating profiles, electrode arrangement in a fully assembled cell [1–3]. However, there is a lack of measurement methods to characterize a single electrode sheet before it is stacked. Access to such information would be very valuable, since one faulty electrode sheet can ruin an entire cell with hundreds of electrode sheets. In this contribution we propose a method to measure the resistance of electrode sheets spatially resolved. The method uses the 4-wire method and can be applied for electrode surface to current collector measurements, or electrode surface to electrode surface measurements for double-side coated sheets. Further, we demonstrate how the gathered measurements can be used on following cases: 1) Identify non-conforming electrode sheets which can subsequently be removed from the manufacturing process, 2) Cluster sheets with similar characteristics to assemble cells of different grades, and 3) identify defects in separator layer of catholyte sheets (cathode and solid electrolyte composite).

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INSTA**BAT** sens**iba**t



BATTERY 2030+ Knowledge Base – Ontologized Standards and Protocols in Battery Research and Development

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The development of standards and protocols in research and development is a key for reaching new levels of cooperation, for complying with FAIR data principles, and for improving the reliability and reproducibility of data and materials generated along the complete battery R&D chain. In the BATTERY 2030+ initiative, we develop and collect standards and guidelines for experimental and theoretical research on batteries as also described in the BATTERY 2030+ Roadmap[1] and make these available to the battery R&D community via an online database. The starting point of our work is a network of key performance indicators (KPIs) and process/measurement parameters (Figure 1, left). This network shows how KPIs and process steps influence subsequent downstream process steps as well as their outputs: Starting with the synthesis of active materials, covering the areas of coating, electrode fabrication, cell assembly and formation, we go all the way to final electrochemical testing. For each individual KPI, we list recommended measuring techniques, available standards and protocols, as well as downstream processes that they will affect. Being fully agile and dynamic, our online database (Figure 1, right) will constantly be expanded and show the complex relations and dependencies of process steps and measurement results on specific KPIs and parameters. Eventually, we hope to arrive at an online knowledge base that brings together the expertise and knowledge of the major battery research centers in Europe and will in particular serve as a valuable educational tool both for aspiring battery scientists and engineers.



Figure 1. BATTERY 2030+ Knowledge Base Website.

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KPI website with easy GUI linked to data base

Machine Learning-Based Analysis of Critical Factors Affecting Performance in Lithium-Sulfur Batteries

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The performance of lithium-sulfur (Li-S) batteries is heavily dependent on materials and cell design due to the complex reaction and degradation mechanisms involved. Consequently, there has been significant research attention focused on improving the performance of these batteries. In this study, we conducted a comprehensive analysis of key factors affecting battery performance, specifically peak discharge capacity and cycle life, using machine learning.

We collected data from 1660 cells in 353 papers from the literature and analyzed them using association rule mining. Our findings indicate that the type and amount of encapsulation material have a critical impact on both high capacity and enhanced cycle life. Furthermore, the use of structured carbons, such as porous carbons or carbon nanotubes, in encapsulated cathodes leads to superior battery performance. We also found that electrolyte design has a significant influence on battery performance, particularly in electrolyte starved cells.

Our results confirm that the most promising pathway for enhancing Li-S battery performance is materials design, specifically the design of encapsulation cathodes and electrolytes that can operate at low electrolyte-to-sulfur ratios and high sulfur loadings. These findings have significant implications for the future development of high-performance Li-S batteries, and they provide important insights for researchers and engineers working in this field.

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Modeling of local electrode stresses and pressures in lithiumion battery packs using three-dimensional homogenization

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During charging and discharging, the electrodes inside the battery cells undergo reversible changes in thickness. These reversible effects are superimposed by an irreversible volume expansion of the electrodes and cells with increased aging. A noticeable change in the thickness of pouch cells/jellyrolls is visible and modeling of swelling behavior becomes crucial for the cell integration inside the battery packs. Lithium-ion batteries have a multiscale structure, which consists of a periodic representative volume element (RVE) consisting of porous electrodes, metallic current collectors, and polymeric separators. There is a coupling between electrochemistry, deformations, and stresses on the scales of active particles, electrode layers, and cells, which makes battery-level simulations computationally very expensive. Here, we present a methodology for the homogenization of battery cells that incorporates a multi-scale approach and integrates layer-level volume expansion into cell-level deformation [1]. The three-dimensional laminate theory is utilized to homogenize the layered structure where each layer is modeled with an experimentally obtained constitutive behavior. The homogenization process is performed using a user-defined constitutive law that enforces the condition of equilibrium and compatibility in the RVE, solves a non-linear set of equations at each integration point, and performs the necessary homogenization of the mechanical quantities. The effects of boundary conditions like external pressure or a stiff casing on the battery level are captured by the homogenized model. With the present methodology, the layerlevel stresses can be back-calculated and highly stressed regions inside the battery can be identified. The model can help decide the range of external pressure and internal stresses/deformations under which the critical structural and electrochemical changes are likely to take effect [2].

In a battery pack simulation, the homogenized cell model can be utilized in conjunction with other battery components such as compression pads, side plates, and thermal pads for faster simulations. To demonstrate the effectiveness of the presented scheme, the homogenized model is applied in finite element software COMSOL on the battery level and the interaction with compression pads and the casing is modeled. The influence on homogenized battery cells from pressure on casing and interaction with compression pads is simulated where the conclusions on layer-level stresses and local pressures are drawn.

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Cell-level Battery Management System for holistic monitoring

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With the growing adoption of batteries on both transportation and power grid, the number of cells deployed has exponentially increased over the years. Consequently, the number of battery-related accidents has increased as well [1]. Battery failures range from economical with systems breaking down earlier than expected, to dramatic with self-ignitions costing lives and millions of \$SU of losses [2].

The leading cause for these accidents is the lack of real-time knowledge of the cell internal state, which is prone to sudden degradation when certain conditions are met [3]. Current battery management systems (BMS) only determine battery state through the monitoring of battery voltage, current, and sometimes temperature, and therefore are unable to accurately determine the internal state of the cells [4].

To solve the shortcoming of current BMS, the SPARTACUS project aimed at adding multiple sensors to each cell of the pack (array of temperature sensor, pressure sensor, ultrasonic, EIS...). However, these additional sensors require a consequent amount of cabling and generate a significant amount of raw data, both of which would not be practical to implement and manage on a classical BMS architecture [5-8], with one single manager monitoring a module of 6 to 20 cells.

As a result, the CSEM within the SPARTACUS project has proposed a new approach to BMS architecture, with the creation of a cell management system (CMS). The CMS is wired to every sensor of the cell, gathers raw data, does the first order processing (e.g. filtering and simple estimator computations), and reports to the battery pack master only post-processed, aggregated data (Figure 1).

The resulting solution is a BMS able to interface to a much higher number of sensors than what is currently possible, in order to gather data from various sensor types, and thus to determine with higher precision the internal state of the cell, leading to a more accurate diagnosis capability, and therefore a safer and more reliable battery pack for the end-user to adopt.



Figure 1. Conceptual(a) and implemented(b) SPARTACUS CMS

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Spray printing of LNMO cathodes with sustainable solvents

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The demand for sustainable and eco-friendly manufacturing processes has become increasingly important, emphasising the field of battery production, where toxic solvents such as N-Methyl-2-pyrrolidone (NMP) are often used [1]. At the same time, spray printing has emerged as a promising approach to producing high-performance, various-shaped batteries, especially from the perspective of solid-state electrolyte implementation [2]. However, the use of toxic solvents in the process has been a concern. Therefore, this study aimed to investigate the use of sustainable solvents for spray printing of cobalt-free high-voltage LiNi_{0.5}Mn_{1.5}O₄ (LNMO) cathodes.

In this study, Cyrene, DMSO, and γ -Valerolactone were tested as alternatives to traditional NMP solvent. The solvents were used to prepare LNMO cathode ink, which was then spray-printed onto an aluminium current collector. The morphology and electrochemical performance of the resulting cathodes were consequently evaluated. The results indicate that the implementation of sustainable solvents requires additional steps related to ink formulation and tuning of the printing process, as these solvents have various properties, such as viscosity, surface tension, and boiling point. Nonetheless, the printed cathodes offer similar performance compared to those produced with NMP. The printed cathodes demonstrate good adhesion to the substrate, uniform morphology, and high electrochemical performance. This study indicates that sustainable solvents are promising alternatives to traditional toxic solvents for spray printing of LNMO cathodes. These findings provide a foundation for the development of more sustainable and eco-friendly manufacturing processes for batteries.

In conclusion, this study highlights the importance of using sustainable solvents in battery production to reduce the impact of manufacturing processes on the environment. The use of sustainable solvents and spray printing in LNMO cathode fabrication is a promising approach to achieving this goal. Future studies will focus on further optimisation of the inks and printing parameters to improve the performance and reproducibility of the cathodes.



Figure 1. a) Spray-printer nozzle. b) Printed LNMO cathodes of various sizes.

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SYNTHESIS OF PIEZOELECTRIC SEPARATOR FOR SELF-HEALING LI-METAL BATTERIES

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Li-metal batteries are considered the next generation of the Li-ion technology, but they will only be enabled if Li loss is avoided at the anode/electrolyte interface. One strategy to be explored is the use of piezoelectric materials to mitigate dendritic growth. In this study, we use a polar polymer to prepare piezoelectric porous separators by non-solvent induced phase separation (NIPS) [1]. This method takes advantage of the polymer's difference in solubility in two different solvents to trigger a phase separation from liquid to solid. This process is visually summarized in Fig. 1(a). The phase separation mechanism yields a microscopic architecture of interconnected pores, see Fig. 1(b). The polar polymer, here polyvinylidene fluoride-trifluoroethylene (PVDF-TrFE), is selected because upon phase inversion from the liquid phase, it spontaneously crystallizes in the polar phase of PVDF, called β -phase, instead of the non-polar α -phase in which usually PVDF crystallizes. We investigate PVDF-TrFE in Li-metal batteries as a potential self-healing material to mitigate lithium dendrite growth [2]. In the framework of the HIDDEN project, the process is scaled up to a roll to roll pilot line. The produced membranes are then compared in full battery configurations as displayed in Fig. 1(c), demonstrating the potential of piezoelectric polymers in mitigating the build-up of dead lithium. This work was performed in the framework of the Battery 2030+ initiative and the affiliated project HIDDEN.



Figure 1. a) Diagram of the NIPS process, b) Cross-section SEM image of the NIPS-produced PVDF-TrFE separator showing the resulting porous structure, c) Li-metal/NMC coin cell cycling with and without PVDF-TrFE separator.

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Re-Parametrization for Model-Based Electrochemical Control

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To use lithium-ion cells on-board electric vehicles (EVs) safely and efficiently, a battery management system (BMS) is essential. It monitors the battery's states and controls the usage by limiting e.g., current and temperature. Advanced BMS use electrochemical models to estimate internal states of battery cells and apply usage constraints based on these [1]. The performance of an electrochemical BMS is closely tied to the performance of the underlying model and the accuracy of its parameters [2].

The parameters of electrochemical models can be identified through physico-chemical characterization techniques, curve fitting [3], or a combination of the two methods. As model parameters change with battery aging [4], re-parametrization of electrochemical models on-board is necessary to conserve model accuracy. Procedures for handling this are an on-going research topic. An attractive option could be identifying model parameters from online measurements during normal operation data. Battery data collected during driving was shown to be informative about Doyle-Fuller-Newman (DFN) [5] model parameters [4]. Alternatively, identification could be based on an informative charging procedure, specifically designed to maximize target parameter sensitivity [6-7]. Informative charging combines the charging task with experimentation by superimposing or interjecting informative current patterns [6-7].

In this work, we study parametrization on optimally designed experiments during charging and conventional driving data. We investigate whether informative charging can improve performance of the DFN model compared to parametrization on driving data. The optimal experiments are designed using global sensitivity analysis and performed throughout an overnight charge. The study is performed on automotive battery cells.

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Deciphering Li deposition and SEI with cryo-EM and cryo-ET

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Understanding in detail the behaviour of Li deposition and SEI formation is crucial for the rational design of stable Li metal anodes, but has remained tremendously challenging due to the extremely high sensitivity of metallic Li. [1] To address this issue, cryogenic electron microscopy (cryo-EM) has in recent years emerged as a powerful tool for visualizing sensitive Li deposition and SEI on the nanoscale. In our study, to understand the morphological evolution of Li nucleation and deposition under various current densities, we performed multiscale morphological characterization of Li deposits and the SEI using cryogenic transmission electron microscopy (cryo-TEM) combined with focused ion beam scanning electron microscopy (FIB/SEM). The Li deposits are found to be ball-shaped where the local charge density is low, while Li-whiskers appear where a high flux of Li-ions and electrons exists. Meanwhile, the Li-balls are concluded to be the origin of the Li-whiskers, and the ball-shaped deposits appear to be mostly amorphous while the Li-whiskers being highly crystalline. Moreover, the nanostructures and compositions of the SEI layer on Li balls and whiskers are different, with thin and LiFdominated SEI on Li-balls and thick and organic-enriched one on Li-whiskers. (Figure 1a) The distinction in SEI is further correlated to the Li nucleation and growth behaviors of these two types of Li deposits. [2] Moreover, to decipher the Li deposition and SEI evolution processes under an operando polymerized SEI which resulted in an ultra-high Coulombic efficiency of 99.97% for Li plating/stripping, we used cryo-TEM and cryogenic electron tomography (cryo-ET), complemented with operando electrochemical atomic force microscopy (EC-AFM), which demonstrated the morphological evolution of Li deposits from large-sized and low-tortuosity spheres to columns, together with thinning of the *operando* polymerized SEI layer from ~100 nm to 7 nm and self-healing capability. leading to efficient Listripping (i.e., with minimum "dead" Li) and non-continuous SEI formation. (Figure 1b) [3] These results provide new mechanistic understandings of Li deposition and SEI growth, which could guide the rational design Li metal anodes and interfaces toward stable operation.



Figure 1. Morphologies of Li deposits and SEI obtained with cryo-EM and cryo-ET.

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Production of highly disordered carbon through CO₂-laser carbonization of polypyrrole/*Cladophora* cellulose free-standing film for energy storage applications

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Worldwide production of carbon materials for various applications reached 10 billion of tons per year. The most popular and widespread method of carbon materials production is pyrolysis. This method requires high temperatures, inert atmosphere and corrosion chemicals for carbonization of biomass, wastes or artificial polymers. Usually pyrolysis takes up to several hours which makes this process low energy effective and expensive. Besides, pyrolysis usually offers weak control on products purity and properties (porosity, microstructure, ordering, surface functionalization and etc.) what limits many applications (e.g. in catalysis and energy) of thus produced materials and makes their production even more difficult. In this work we showed that CO₂-laser irradiation of material with high absorption coefficient can be used as sustainable, fast and scalable method for carbon materials production. The polypyrrole-coated *Cladophora* nanocellulose fiber was used for creation of free-standing photothermal film which further was successfully carbonized by CO₂-laser irradiation during several minutes on air. The structure and functional composition of formed carbon material was probed using SEM-EDX, XPS, FTIR methods. We showed that morphology, microstructure, functional composition and porosity of the material strictly depends on the parameters of the irradiation as well as carbonization degree. The specific capacity of the material reached ~ 145 F g⁻¹ at 1 mV s⁻¹ scan rate in 2M NaOH aqueous electrolyte. Moreover, material provide prominent areal capacitance in order of ~ 62 μ F cm⁻².



Laser-induced carbonization vs. pyrolysis

Figure 1. The comparison of two approaches for carbon materials production for energy storage applications.











Investigations of oxygen flow rate on Li – O₂ battery discharge capacity and design of rotating ring disk electrodes for OER/ORR electrocatalysts

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Lithium-oxygen (Li-O₂) batteries have a high theoretical energy density and capacity compared to other rechargeable batteries, which makes them potential candidates for the next generation of commercial batteries [1]. To optimize the performance of Li-O₂ batteries an optimal design for controlling the oxygen flow rate is critical. In this investigation, the effects of varying oxygen flow rates on the capacity of $Li-O_2$ batteries were studied. The experiment was carried out using a conventional Li-O₂ battery setup equipped with oxygen flow rate controllers to be able to vary the O₂ flow in the inlet. The cells consisted of conventional lithium metal as the anode, a carbon paper gas diffusion layer (GDL) with a microporous coating as the air cathode and a double layer of fiberglass as the separator, and 1 M LiTFSI/TEG-DME electrolyte. The battery's capacity was measured under different oxygen flow rates in an open system. The results were analyzed to determine the optimum conditions for maximizing battery capacity. Our results show that low oxygen flow rates increase the battery's discharge capacity compared to high O₂ flow rates, varying from 615 mAh g⁻¹ to 835 mAh g⁻¹ at a flow of 1.0 L min⁻¹ and 0.05 L min⁻¹, respectively. This agrees with a previous study carried out under slightly different conditions [2]. Despite that higher flow rates provide more oxygen to react with lithium ions, a higher oxygen flow rate may cause the battery to degrade more quickly, as the oxygen can react with other components in the cell. In the next part of the project, we demonstrate how to construct two different types of rotating ring disk electrodes (RRDE) electrodes. We compare the standard commercial RRDE design with and rotating acentric disk-disk electrode (RADDE) recently reported by Qi et al [3]. We evaluate parameters such as collection efficiency, sensitivity factor, and current/product responses, with respect to internal parameters (r1 and α) of the electrodes. We further employ these electrodes to study the electrochemical activity of common metal electrocatalysts for oxygen evolution and reduction (ORR/OER) reactions [4].



Figure 1. a) Discharge curves of the Li-O₂ cell in different oxygen flow rates. The inset shows the flow rate control station. b) Design and assembly of a standard rotating ring disk electrode (RRDE) and a rotating acentric disk-disk electrode (RADDE).

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Understanding the reactivity of organosilicon additives with water under battery conditions

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The use of organosilicon-containing additives in lithium-ion battery (LIB) electrolyte engineering has received considerable attention due to their multifunctional properties. Tris-(trimethylsilyl)phosphate (TMSPa), a prominent member of this class of additives, has been shown to scavenge Lewis base like water; ¹ however, the reaction rate and fate of the resultant product in the battery system are not well understood. In this study, we used complementary nuclear magnetic resonance (NMR) and gas chromatography-mass spectrometry (GC-MS) to systematically investigate the reactivity of TMSPa with water in a typical carbonate solvent-based environment. We identified the reaction products and proposed a working reaction pathway by tracking the chemical evolution of the products at varying time and temperatures. Our findings revealed that the main reaction products were trimethylsilanol (TMSOH) and phosphoric acid (H₃PO₄), along with various other P-O-Si containing intermediates. TMSOH can undergo polymerization at room temperature to form hexamethyldisiloxane (TMSOTMS) and can also activate ethylene carbonate (EC) ring-opening reactions at elevated temperatures (≥80 °C) yielding TMS derivative ethylene glycol (TMS-EG). Although the formation of TMS-EG at the expense of EC is an unwanted parasitic reaction, this reaction is only activated at elevated temperatures compared to EC ring-opening catalyzed by H2O, which occurs at \geq 40 °C.² This study highlights the superiority of TMSPa as an electrolyte additive, and elucidating the reaction mechanism is essential for future studies of such additives to improve the accuracy of additive exploration in LIBs.



Figure 1. Figure: ²⁹Si NMR spectra showing chemical reaction products of TMSPa with H₂O in carbonate-based solvent system at two different temperatures (30 and 60 °C).

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Prospective environmental impacts of a smart battery cell

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The spatially resolved acoustic, mechanical, and ultrasonic sensing for smart batteries (SPARTACUS) project targets developing smart battery cells with affordable sensor solutions to detect failure mechanisms before performance loss. This study assesses the environmental impacts of the smart cell compared to a state-of-the-art (SoA) cell based on a prospective life cycle assessment (LCA).

The system boundaries include the extraction of the raw materials, manufacturing of the cell and the sensors and the use stage. The functional unit is 1 kWh of delivered energy. The prototype contains 3 polyimide (PI) layers (PI#2, PI#3, and PI#4) on a commercial 12 Ah pouch cell. Acoustic sensors are placed on PI#2 and PI#3 to identify material changes in the cell. PI#2 also contains temperature sensors. On PI#4, rubber compression sensors monitor deformation by detecting mechanical stress and pressure distribution. A cell management system (CMS) and a pre-processing (PP) board are also included.

Data for the manufacturing stage is as much as possible primary, obtained on a lab scale. Data for the use stage is real data from tests of SoA cells based on the Worldwide Harmonised Light Vehicles Test Procedure (WLTP) cycles. The prototype is assumed to have a 20% longer cycle life. The life cycle impact assessment is conducted using IPCC GWP100a characterization factors. The prospective LCA assessed climate change impacts in 2030 and 2050, with 2020 as the reference year. The scenarios are based on the SSP2-base and SSP2-RCP 2.6 (2°C climate target), thanks to a prospective superstructure database [1].

The impact on climate change of the prototype is at least 160% higher than the SoA battery cell in all scenarios (Figure 1). Including the future developments of the background database reduces the impacts in ten years. In all years and scenarios, most of the impact comes from PI#4 (23% of the total contribution), followed by PI#2 and PI#3 (both contributing with 14%). In 2030, in the RCP 2.6 scenario, the impacts of the prototype are reduced by 21%.



Figure 1. Impacts on climate change of the cells in 2020 and 2030, based on the base and Representative Concentration Pathway (RCP) 2.6 scenarios. Legend: CMS = cell management system, PI = polyimide, PP = pre-processing, SoA = State-ofthe-art.

The large impact increase due to the sensors indicates the need to identify sensors that can be excluded from the prototype to reduce its life cycle environmental impacts. Therefore, future development includes including the full life cycle with recycling to support a better understanding of the contribution of the environmental impacts of the sensors.

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Selected Lecture Abstract





SPARTACUS Project: How to make batteries smart by optimized sensor technologies

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The SPARTACUS project aims for the use of acoustic-mechanical sensors and their non-invasive integration on battery cells to measure defects and degradations in the battery with a local resolution. The knowledge about the State of Health (SoH) can be used to optimize the charging profile. This results in accelerated charging cycles without shortening the battery lifetime.

The project adapts different kind of sensors, such as e.g., temperature sensors, ultrasonic sensors [1] and strain sensors in order to measure thermal changes, changes in the Young's Modulus and thickness. All sensor devices can be used in order to determine the state of charge showing the relevant electrochemical processes during cycling. The sensor portfolio is completed by Odd-Random-Phase Enhanced Impedance spectroscopy that gives additional insight into the electrochemical processes of the battery cell.

The sensors are implemented by means of scalable processes that make the technological approach suited for industrial manufacturing. Therefore, sensors are assembled on polyimide sheets; Conductors are printed in order to generate the wiring between the sensors and connectors. Conventional assembly techniques such as Pick & Place is used in order to set the temperature sensors in the right place.

The contribution describes the progress in the data preprocessing in order to be able to interpret the data correctly and to make them available for cell and battery management systems. Different aging campaigns were started in order to provoke degradation effects and to correlate those to the corresponding sensor signals. Aged batteries are investigated by post-mortem analysis in order to assign the sensor signals to the respective degradation effects.

Based on these investigations, SPARTACUS build up models that form the base for the battery management system in order to control the battery cycling. For validation, test set-ups were prepared in order to prove that the sensor technology enhance the battery performance. Different kind of models based on machine learning approaches are trained in order to evaluate the high number of data generated. Cell and battery management systems CMS/BMS) are developed and realized on a hardware level. The CMS uses the models and sensor data. Finally, the smart batteries are validated by accelerated testing methods using harmful cycling profiles at different temperature regimes.

An accompanied LCA and cost assessment is carried out in order to get a first indication about the effects of the equipped battery on sustainability and economics. Thereby, most critical materials and components can be identified that have a negative effect for both, economic and ecologic aspects. Based on the findings of SPARTACUS project, sensor technologies can be designed in a way that most relevant sensor data can be generated with a set of sensors as small as possible in order to increase the sustainability and the economics.

The contribution also highlights the battery 2030+ roadmap and the contribution of SPARTAUS towards the roadmap objectives.









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Figure 1. Smart battery instrumented with different kind of sensors.

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Cell-integrated Sensing functionalities for smart battery systems with improved performance and safety

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The objective of the present study is to develop a sensing technology for Li-ion batteries that measures in realtime the internal battery cell temperature, pressure (e.g. mechanical strain, gas evolution) conductivity and impedance (separately for the anode, cathode and electrolyte). The data and insights from these new sensing technologies are used for the development of improved state estimator functions based on an improved understanding of how, where and when degradation and failure mechanisms occur. These functions are included in the BMS.

The approach consists of five steps:

1) develop the sensor technology

2) integrate this sensor technology into 1Ah and 5Ah pouch battery cells

3) incorporate the cells in a module BMS,

4) use the data from the internal sensing technologies to develop robust and advanced state estimation functions. Several state (SOC/SOH/SOE/SOP) estimation algorithms will be improved, better forecasting algorithms and novel safety concepts (SOS) will be created,

5) carry out a cost-benefit analysis for the batteries with sensors as well as a recycling study of the cells.





Figure 1: developed internal temperature and preassure sensor, integration of the sensor in the 1 Ah pouch cell and comparison of 1Ah cells with and without integrated sensor

Improved understanding about the nature and timing of unwanted internal battery processes enables faster and more accurate control of the individual cells in a battery system during operation.

More accurate control stretches the possibilities of fast charging and discharging, increases the usable battery capacity and therefore range in different weather conditions and gives a detailed usage history. It allows for better battery state forecasting, resulting in a longer lifetime and more economical use during its 1st and 2nd life. Sophisticated lifetime prediction models enable improved (preventive) maintenance schemes.

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SMART BATTERY FROM SENSING TO BMS: INSTABAT OVERVIEW

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The research goals on development on smart cells are one of the three pillars of the Battery 2030+ roadmap **[1,2]**. Increasing the performance, lifetime and safety of cells require monitoring internal parameters to define the new State of X (SOX) for the cells (state of power, state of health, and state of safety). To achieve these goals, the development of new sensors technologies for in situ and operando are required.

INSTABAT project [3] is a European project started in 2020 under the umbrella of the EU BATTERY 2030+ largescale initiative. The project ambition is to address the short-term BATTERY2030+ roadmap goals for smart cells. For that, we develop a proof of concept of smart sensing technology embedded in the cells to monitor internal physical and chemical key parameters of the cell. During the project, we develop a concept of "lab-on-cell" based on new embedded physical and virtual sensors to perform reliable and in operando monitoring of these key parameters. This monitoring is used to improve the performance and safety thanks to enhanced Battery Management Systems algorithms and real-time higher accuracy SOX determination. After an overview of INSTABAT project, the recent results of the project will be presented with a focus on the results on internal cell parameters measurement by physical sensors. We also highlight the results on the development of virtual sensors and how we improve the SOX indicators. By these examples, the presentation will give an overview of the "Lab on cell" concept developed all along the INSTABAT project.



Figure 1. Synoptic of INSTABAT project, the Lab-on-cell concept.

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YOUNG SCIENTISTS EVENT

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The BATTERY 2030+ community called young scientists to participate the young scientist event, organized on June 1st 2022, across four European cites simultaneously (POLITO Politecnico di Torino, UU Uppsala University, Vrije Universiteit Brussels VUB, Warsaw University of Technology WUT). This event aimed to engage young scientists to write the "Manifesto for batteries of the future" (https://battery2030.eu/news/activities/young-scientist-manifesto/) where they expressed their ideas about the future battery research landscape by providing input on the BATTERY 2030+ roadmap and curricula. The scientists were selected in order to gather a wide range of experience and competences, both within and outside the battery field.

The young scientists of different expertise were sitting around tables to discuss the future outlook of the European battery research and expectations.

People participating were of different expertise, i.e. battery experts, engineers, chemists, physicians, economists, doctors in medicine, people with all humanistic specialisations, etc.

120 people participated in presence: 50 in Torino, 30 in Uppsala, 20 in Brussels and 20 in Warsaw.

The Manifesto was presented in many events and it is one of the young scientists engagement activities. The general assemblies of Battery2030 are additional events.



Figure 1. the Young Scientists











From R&D approach to Industrialization of Single Ion Monomers & Polymers

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Power delivery of Solid Polymer Electrolyte materials is limited by the concentration gradient of the lithium salt, resulting in a low lithium transference number. Traditional electrolytes are dual-ion conductors, i.e., both cations and anions are mobile in the polymer electrolyte phase. The mobility of both ions induces a concentration polarization and finally ends up reducing electrolyte performance.

Single lithium-ion conducting polymer electrolyte, consists of immobilizing the lithium counter ion to the polymeric material. This exceptional single ion transport behavior in combination with their solid-state nature, flexibility and processability brings remarkable benefits to battery structure and performance.

In 1996, M. Armand et al [1] discovered the interest of unsaturated perfluorinated amides salts (e.g. LiTFSI) and their uses as ionic conductive materials.

For 6 years, SPECIFIC POLYMERS proposed to the whole R&D Battery community TFSILi based Monomers & Polymers : MTFSILi (SP-49-023) and STFSILi (SP-59-011), PMTFSILi (SP-4P-6-004) and PSTFSILi (SP-5P-9-009).

These 4 products are of great interest for the R&D community [2] [3] [4] [5], and it is time for SPECIFIC POLYMERS to talk about all the steps that remains to be validated to start the industrialization of these Single Ion Monomers & Polymers.

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Multiphysics Modelling of BAT4EVER Cells: From Parameters to 1D Isothermal Models

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BAT4EVER Project focuses on integrating the self-healing functionalities into the battery components namely electrodes and electrolytes through self-healable binders and polymerized ionic liquids (Figure 1).



Figure 1. BAT4EVER Approach on a) Silicon anodes and b) NMC cathodes

This ambitious project covers an extensive experimental work in combination with complementary multi-scale modelling activities targeting to narrow the gap between application and concept. Within the scope of the BAT4EVER project, Multiphysics modelling will start from Single Particle Model (SPM) development and validation. As a next step, complexity will be added and 1D models will be validated. The models will be realized under isothermal conditions [1].

In this work, we report the recent advances for the Multiphysics based electrochemical modelling in the BAT4EVER project. The parameters necessary to properly develop models will firstly be discussed. After that, the experimental protocols to obtain the parameters is discussed. Finally, the obtained parameters will be implemented into the Multiphysics-based software called COMSOL Multiphysics Battery Design Module. During electrochemical modelling, optimization will also take place by using COMSOL Optimization Module [2].

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OPERA: DEVELOPMENT OF OPERANDO TECHNIQUES AND MULTISCALE MODELLING TO FACE THE ZERO-EXCESS SOLID-STATE BATTERY CHALLENGE

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Green, high-performing and safe batteries based on abundant materials are a key element in the transition to a carbon-neutral future. However, to accelerate their development, a deep understanding of the complex electro-chemo-mechanical processes within the battery is required, which is only accessible through advanced experimental and computational methods. Zero-excess solid-state batteries, where the anode is formed in situ, have emerged as a promising new generation of environmentally friendly batteries with high energy density, improved safety and higher cost-efficiency, but only after solutions for non-uniform anode formation were found.

In OPERA, seven leading research institutions, two synchrotron radiation facilities, a small-medium sized enterprise and a large technological company, all from complementary research fields such as batteries, surface and material science, and multiscale modelling, propose a unique strategy to face the current challenges of this technology. OPERA relies on the development of novel operando experimental techniques at the ESRF, ALBA and DESY synchrotrons and at the lab-scale, providing complementary information on multiaxial stress fields, chemical composition, nucleation and growth kinetics, structural defect formation and degradation of well-defined model cells with a resolution down to the atomic scale. The new insights and collected multiparameter data will be incorporated into a novel multiscale modelling approach supported by machine learning algorithms. This will ultimately lead to a conceptual understanding of the in-situ anode formation and, based on this, innovative improvement approaches to enable this type of energy storage technology, which will be an important step towards increasing the global competitiveness, resilience, and independence of the EU.



Figure. Diagrams of the main high spatial resolution operando techniques proposed in OPERA: (a) CSnanoXRD, (b) PEEM, (c) TEM and (d) SPM.



Thank you for participating in this year's BATTERY 2030+ Annual Conference!



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