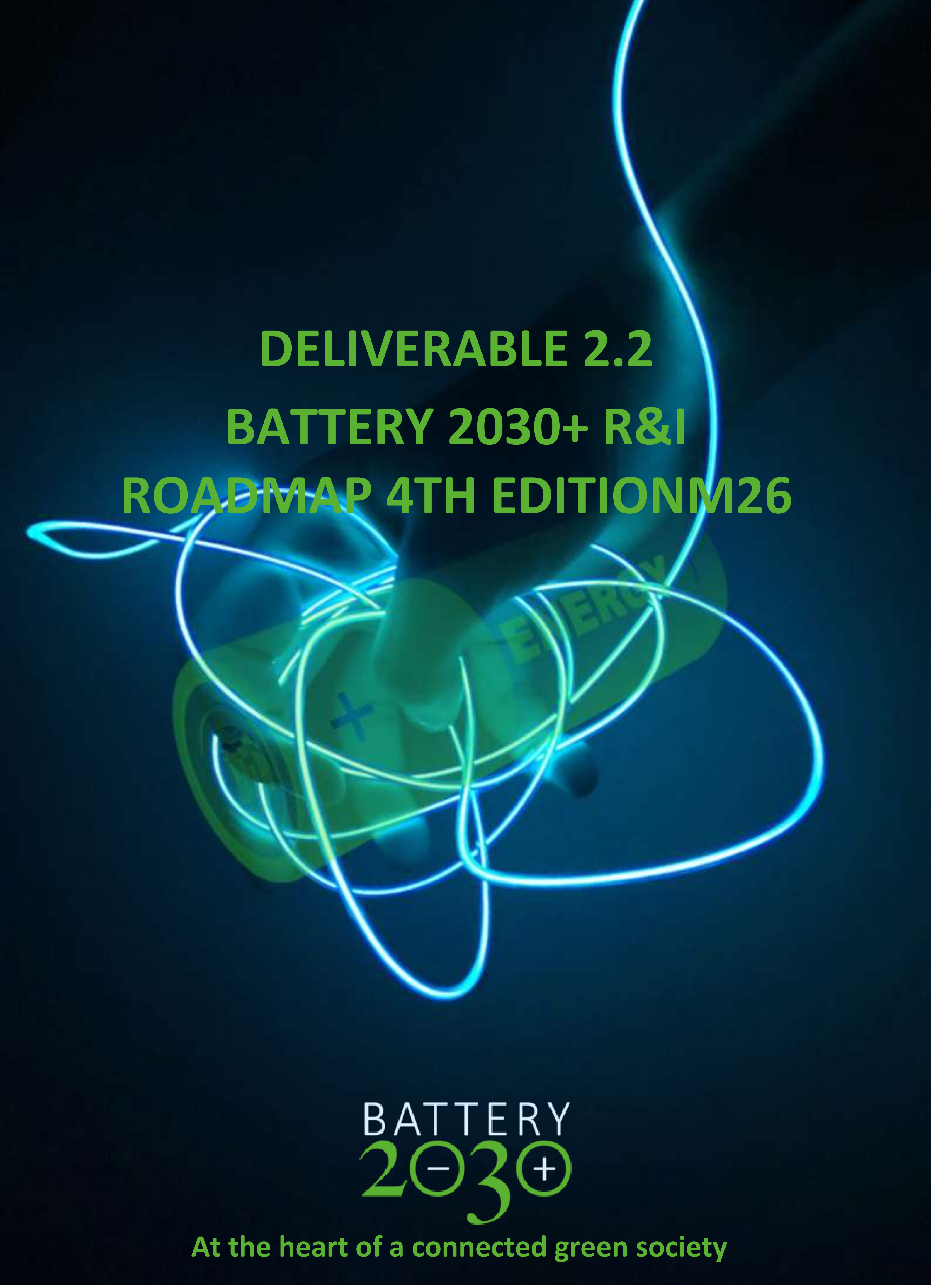

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BATTERY 2030+

At the heart of a connected green society

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INTRODUCTION

Battery technology is a cornerstone of European energy security and prosperity. Since the first modern battery was invented in Europe more than 200 years ago, batteries have become an essential part of our everyday lives, powering our phones, our transportation, and our electricity grid.

But now the world is changing. The energy landscape is becoming more diverse; the global economy and supply chains are evolving; and battery technology must also adapt to remain competitive and meet our future needs.

The rapid development of lithium-ion batteries (LIBs) transformed many technological domains. We must also develop other chemistries to avoid over-reliance on certain materials and over-exposure to risks. A fundamental transformation of battery technology is required which strengthens the foundations of an independent European energy economy.

Europe's diffuse battery research and industrial landscape faces growing challenges and intensifying global competition, particularly from China and the United States[1]. Battery 2030+ offers a strategic response to unify and accelerate European efforts.

Offering Interdisciplinary Coordination and Support

Battery 2030+ is a Coordination and Support Action (CSA) that unites and amplifies the impact of multiple large-scale research projects advancing the next generation of battery technologies. It provides cross-cutting resources, frameworks, and communication channels to ensure coherence, knowledge exchange, and strategic alignment across the European battery research landscape.

Battery research and innovation are inherently interdisciplinary, spanning topics like fundamental materials science, engineering, manufacturing, and policy making. To achieve true European leadership, these diverse efforts require a clear and coordinated approach that unites them toward shared goals and vision. Battery 2030+ and its associated projects pursue exactly that: a bold, multidisciplinary strategy that connects materials discovery, digital technologies, and advanced manufacturing in an integrated framework. This approach accelerates innovation and ensures that breakthroughs in research translate effectively into industrial and societal impact.

Battery 2030+ aligns closely with European policy frameworks such as the European Green Deal[2], the Strategic Energy Technology Plan (SET Plan)[3], and the evolving EU Battery Regulations[4]. Aligning scientific and technological progress with policy objectives is essential to ensure that research outcomes directly support Europe's climate goals, regulatory priorities, and industrial competitiveness. It is strongly committed to a circular economy, designing batteries from the outset for sustainability, ease of recycling, and reuse, supported by advanced sensor and functional technologies and a data-driven digital infrastructure.

Since its launch, Battery 2030+ has continuously built upon successful projects such as BIG-MAP, to foster open collaboration, standardization, and cross-sector integration, providing a strong foundation for Europe's continued leadership and future breakthroughs in battery research and innovation.

The Destination: A Vibrant Battery Innovation Ecosystem

At the heart of Battery 2030+ lies a bold vision: to establish a closed-loop innovation ecosystem that seamlessly connects materials discovery, design, manufacturing, and recycling into one continuous,

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[1] Ahlgren, P., et al., BATTERY 2030+ and its research roadmap: A bibliometric analysis. ChemSusChem, e202300333, 10.1002/cssc.202300333 (2023).
[2] https://commission.europa.eu/strategy-and-policy/priorities-2019-2024/european-green-deal_en
[3] https://energy.ec.europa.eu/topics/research-and-technology/strategic-energy-technology-plan_en
[4] https://environment.ec.europa.eu/topics/waste-and-recycling/batteries_en

data-driven process. This vision represents a fundamental shift away from today's linear research and production chains towards an intelligent, self-reinforcing system where knowledge and data flow in both directions across the battery lifecycle.

Achieving this vision is essential for Europe to accelerate battery innovation, reduce development time and cost, and ensure sustainable, circular value chains. By closing the loop between discovery, production, and end-of-life management, Europe can maintain global competitiveness while meeting its climate and resource-efficiency goals.

When fully realized, this integrated ecosystem will enable Europe to overcome many of the limitations that constrain today's battery technologies. It will help increase energy density by optimizing how materials scale from the laboratory to full cells and packs. It will extend lifetime and reliability through advanced materials, embedded sensors, and self-healing functionalities that allow batteries to monitor and repair themselves. It will improve power and fast-charging capability by enhancing ion transport and cell architectures, while simultaneously addressing critical safety challenges associated with rapid cycling and extended use. Moreover, it will establish manufacturing processes that are inherently circular, cost-effective, and compatible with large-scale recycling and reuse.

To realize this vision, Battery 2030+ integrates digital and experimental advances across disciplines. AI-driven Materials Acceleration Platforms (MAPs) and the Battery Interface Genome (BIG) enable rapid discovery and optimization of materials and interfaces. Embedded sensors generate real-time data that feed predictive models, enabling both preventive and adaptive self-healing within batteries. Manufacturing processes incorporate these insights to embed self-healing capabilities and are designed from the outset for recyclability. Digital twins connect design, production, operation, and recycling data, ensuring continuous feedback and optimization throughout the lifecycle. Together, these efforts form the foundation of a truly European ecosystem for smart, sustainable, and circular battery innovation.

Figure 1 illustrates the integrated structure and interconnections across these thematic areas, providing a clear overview of the strategic framework. The closed-loop approach forms the foundation for broad industrial and societal impact, shaping how Europe designs, manufactures, and uses batteries to achieve its energy and climate goals.

The Battery 2030+ Roadmap: A Long-Term Vision for Success

This Roadmap is structured into seven thematic areas:

Accelerated Materials Discovery provides the methodological basis for faster and more reliable development of new materials. By combining automation, modelling, and data-driven approaches, Europe can reduce reliance on trial-and-error research and shorten the time to implementation.

The Battery Interface Genome addresses one of the central bottlenecks of advanced batteries: the complexity of interfaces and interphases. Understanding and controlling interfacial processes is key to improving safety, stability, and lifetime, especially for emerging chemistries.

Sensing and self-healing, smart management, and digital twins, enhance the operational reliability of batteries. By embedding monitoring and repair mechanisms, failure rates can be reduced, service life extended, and safety improved. These functionalities not only enable proactive battery management but also generate valuable data to support predictive maintenance.

The theme of **New Chemistries and new technologies** explores alternatives to current lithium-ion systems. These include sodium-ion, solid-state, multivalent, metal–air, and organic batteries. Each is assessed with respect to sustainability, scalability, and application relevance, ensuring that resources are directed toward options with clear added value.

Manufacturing and Digital Twins focuses on how new materials and chemistries can be translated into industrial practice. Digitalisation of manufacturing processes improves efficiency, reduces waste, and enables flexibility in production lines — an essential requirement for adapting to new chemistries and functionalities.

The area of **Recycling and Circularity** ensures that design and production choices take end-of-life into account from the outset. Direct recycling, reconditioning, and second-life strategies are central to establishing a circular battery economy and reducing Europe's dependence on critical raw material imports.

Finally, **Data, standards and ontologies** provide the tools for ensuring quality, interoperability, and reproducibility across all activities. Shared infrastructures, ontologies, and protocols are essential for collaborative research and for efficient transfer of knowledge into industrial applications.

Together, these seven areas form a comprehensive and coherent Roadmap. Each addresses a critical element of the battery research and innovation landscape, and their combined implementation aims to help Europe reach its long-term goals of technological sovereignty, climate neutrality, and industrial competitiveness.

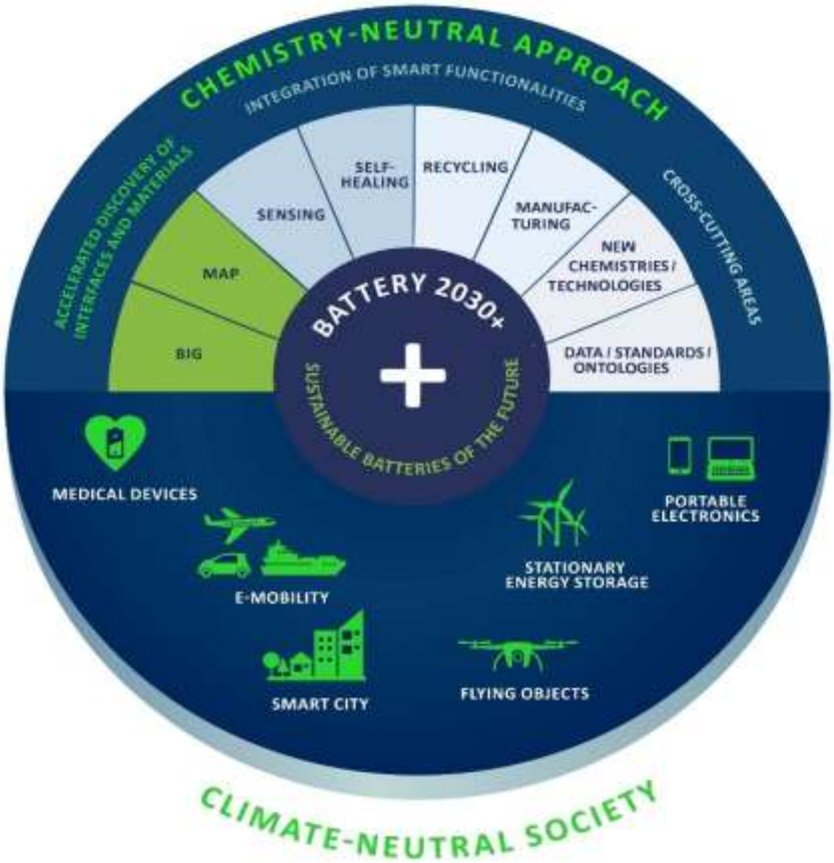

FIGURE 1. Integrated Structure of Battery 2030+

1. ACCELERATED MATERIALS DISCOVERY

Battery 2030+ aims to dramatically speed up how new battery materials are discovered, tested, and optimized. Accelerated Materials Discovery is the cornerstone of this effort: it replaces slow, trial-and-error experimentation with fast, automated, and data-driven workflows that continuously learn and improve over time. This new paradigm is essential to meet the growing demand for sustainable, high-performance materials that can power Europe's clean energy future.

At the heart of this vision is the modular, interoperable Materials Acceleration Platform (MAP) - a system that combines automated experimentation, multiscale modelling, and AI-driven data analysis into self-improving, closed-loop workflows. The concept builds on the foundations laid by the BIG-MAP project (2020-2024), as presented in detail in the third edition of the Roadmap published in 2023[5].

The current Roadmap focusses on modularity, generalization, and interoperability, ensuring the development of a distributed European network of interconnected MAP nodes with shared protocols, data, and workflows. These MAPs leverage autonomous, "self-driving" laboratories[6] for High-Throughput (HT) materials synthesis, characterization, computational modelling, and autonomous data analysis, accelerating the discovery, testing, and optimization of battery materials, interfaces, and cells.

Building on key infrastructures such as the *FINALES*[7], Bue[8], HELAO, *AURORA* lab automation[9], MADAP, and BattINFO, the new FULL-MAP project (2025–present) now implements these capabilities in practice across nine diverse battery chemistries and use cases. FULL-MAP is still in its early stages, and full deployment of automation, semantic integration, and cross-platform interoperability has yet to be achieved.

1.1 Introduction

Battery 2030+ defines a new path for the accelerated discovery and rapid development of ultra-high-performance, sustainable, and intelligent batteries[10]. This chapter outlines the opportunities, challenges, and current status of establishing a community-wide European battery Materials Acceleration Platform (MAP) that will be integrated with the Battery Interface Genome (BIG) described in the following chapter.

The emerging discovery framework and shared data infrastructure[11], as initially developed in the BIG-MAP project, demonstrated that a modular, interoperable, and versatile approach can accommodate all current and future battery chemistries, materials, and interfaces. Inspired by earlier international efforts such as the Materials Genome Initiative[12] and following the format of Mission Innovation: Clean

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[5] https://battery2030.eu/wp-content/uploads/2023/09/B-2030-Science-Innovation-Roadmap-updated-August-2023.pdf

[6] Seifrid, M. *et al. Routescore: Punching the Ticket to More Efficient Materials Development.* Cambridge University Press (CUP) (2021).

[7] Monika Vogler. et al., Autonomous Battery Optimization by Deploying Distributed Experiments and Simulations. Advanced Energy Materials, 202403263, (2024).

[8] Simon K. Steensen, et al., The Necessity of Dynamic Workflow Managers for Advancing Self-Driving Labs and Optimizers, Advanced Intelligent Discovery, 202500067, (2025).

[9] Monika Vogler. et al., Brokering between tenants for an international materials acceleration platform. MATTER, 10.1016/j.matt.2023.07.016 (2023).

[10] Bhowmik, A. *et al.* Implications of the BATTERY 2030+ AI-Assisted Toolkit on Future Low-TRL Battery Discoveries and Chemistries. *Advanced Energy Materials*, 2102698, 10.1002/aenm.202102698 (2021).

[11] Castelli, I.E., *et al.,* Data Management Plans: The Importance of Data Management in the BIG-MAP Project (2021), https://arxiv.org/abs/2106.01616.

[12] NATIONAL SCIENCE AND TECHNOLOGY COUNCIL, Materials genome initiative strategic plan (2021), https://www.mgi.gov/sites/default/files/documents/MGI-2021-Strategic-Plan.pdf.

Energy Materials (Innovation Challenge 6) MAP Roadmap[13], MaterialsCommons4EU[14], and further conceptual iterations[15], BIG-MAP concept combines automation, robotics, artificial intelligence, and machine learning to orchestrate data acquisition and utilization across complementary experimental and computational techniques (See Figure 2).

Realizing the full potential of this battery MAP framework still requires major advances in automation, data infrastructure, and AI-driven coordination. These enabling technologies underpin a new battery development strategy based on inverse design, which pursues the targeted creation of materials, interfaces, and devices from desired properties rather than empirical trial and error. When fully coupled, all MAP components will form AI-orchestrated, autonomous discovery workflows, dramatically accelerating development speed, improving performance prediction, and enhancing safety assessments[16].

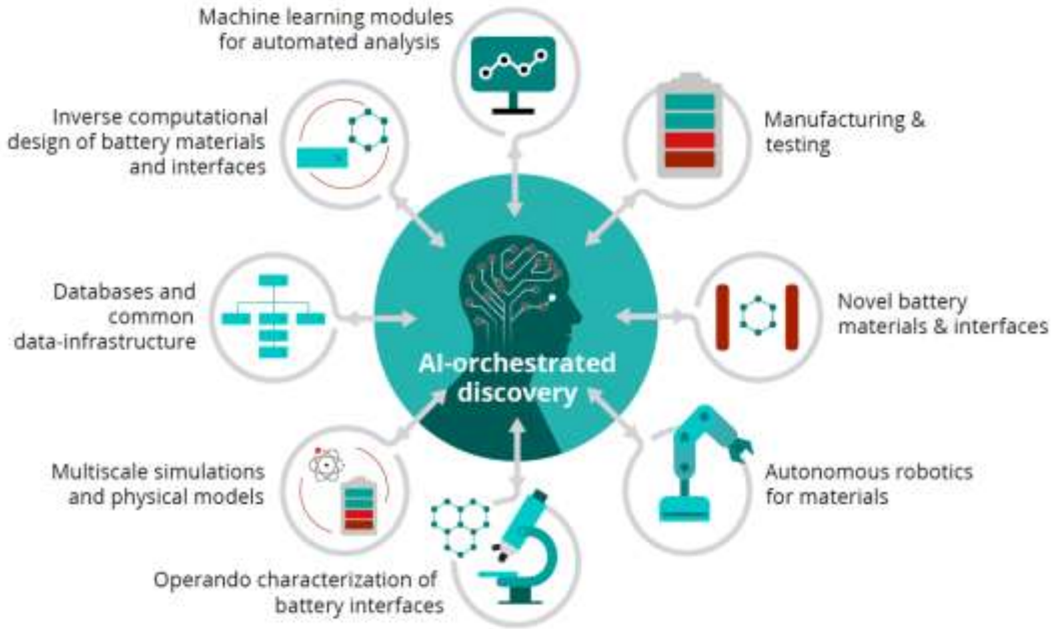

FIGURE 2. Key components of establishing the battery Materials Acceleration Platform in BIG-MAP (www.big-map.eu).

The successful integration of computational materials design, AI orchestration and machine learning, modular and autonomous synthesis, robotics, and advanced characterization will be the foundation for transforming the traditional, sequential materials discovery process into a rapid, self-improving, closed-loop system[17].

1.2 Current Status

For decades, the development of new battery materials has followed an Edisonian, or trial-and-error, approach in which progress along the discovery chain depends on the completion of each preceding

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[13] Clean Energy Materials Innovation Challenge Expert Workshop, Mission Innovation, Clean Energy Materials Innovation Challenge (IC6). Materials Acceleration Platform-Accelerating Advanced Energy Materials Discovery by Integrating High-Throughput Methods with Artificial Intelligence (2018), http://mission-innovation.net/wp-content/uploads/2018/01/Mission-Innovation-IC6-Report-Materials-Acceleration-Platform-Jan-2018.pdf.

[14] https://materialscommons4.eu

[15] Davydov, A.V., Kattner, U.R., Predicting synthesizability. *Journal of physics D: Applied physics.* **52,** 10.1088/1361-6463/aad926 (2019).

[16] Vegge, T., *et al*. Toward Better and Smarter Batteries by Combining AI with Multisensory and Self-Healing Approaches. *Advanced Energy Materials*, 2100362, 10.1002/aenm.202100362 (2021).

[17] Lombardo, T. *et al.,* Artificial Intelligence Applied to Battery Research: Hype or Reality? *Chemical Reviews,* 10.1021/acs.chemrev.1c00108 (2021).

step. This sequential process has yielded many breakthroughs but remains time-consuming, labour-intensive, and difficult to scale.

In recent years, several individual steps have been partially automated or digitally integrated, but progress toward full autonomy and closed-loop discovery has so far been incremental[18]. Examples include electrolyte formulation, full battery cell assembly [19] end-of-line characterization, rapid experiments in half-cell setups, and hyperspectral mapping capabilities.

Through the development of initiatives like FINALES[20], these systems are now being integrated with machine learning, multi-scale computational material design, and operando characterisation techniques in a circular design loop, laying the groundwork for truly autonomous, self-improving discovery workflows.

However, additional layers of interoperability and further acceleration are needed to reach the highly ambitious goals of Battery 2030+, especially when it comes to various battery prototype options and material design and synthesis routes. Making these accessible for a wide range of high-throughput optimisations require a synergetic and wider material approach on the EU scale.

Ideally, such a circular materials development process should integrate experimental and theoretical research in a closely coupled development platform that enables near-instantaneous cross-fertilisation of the results of complementary techniques, carefully defining performance, and characterisation proxies to measure the optimised battery structures and materials. In the following sections, we summarise the state of the art in key areas of MAP.

Interoperable data infrastructures and ontology-based databases are cornerstones of accelerated, rational battery design. They ensure that high-quality, Findable, Accessible, Interoperable, and Reusable (FAIR) data from experiments, testing, and modelling can be accessed, shared, and integrated across scales and disciplines. Achieving this level of interoperability is essential to connect the growing volume of multi-sourced and multi-fidelity data generated by autonomous laboratories, high-throughput (HT) simulations, and large-scale experiments.

Globally, initiatives such as the Materials Genome Initiative in the United States and the Materials Cloud[21] in Europe aim to create flexible and shareable databases and repositories[22,23] for experimental data. In parallel, computational infrastructures such as PRACE and EuroHPC, and platforms such as PerQueu[24], SimStack[25], and AiiDA[26] facilitate workflows[27] for efficient and reliable HT calculations, while only few examples like the OPTIMADE[28] REST API bridge computational and experimental data.

Within Europe, recent efforts are building battery-specific data infrastructure, designed to accommodate heterogeneous multi-sourced datasets envisioned here. To fully exploit these data, extensive efforts e.g., by the European Materials Modelling Council (EMMC)[29] have been made to

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[18] Fichtner, M. *et al.,* Rechargeable Batteries of the Future-The State of the Art from a BATTERY 2030+ Perspective. *Advanced Energy Materials*, 2102904, 10.1002/aenm.202102904 (2021).
[19] Enea Svaluto-Ferro., *et al.* Toward an Autonomous Robotic Battery Materials Research Platform Powered by Automated Workflow and Ontologized Findable, Accessible, Interoperable, and Reusable Data Management. *Chemistry Europe. DOI: 10.1002/batt.202500155* (2025)
[20] Vogler, M. *et al. Brokering between tenants for an international materials acceleration platform* (2022).
[21] Materials Cloud – A Platform for Open Science, https://www.materialscloud.org/home.
[22] The Novel Materials Discovery (NOMAD) Laboratory., https://nomad-coe.eu/.
[23] The EUDAT Collaborative Data Infrastructure, https://eudat.eu/.
[24] https://pubs.rsc.org/en/content/articlelanding/2024/dd/d4dd00134f
[25] SimStack – Computer-Aided Molecule Design, https://www.simstack.de/.
[26] Pizzi, G., Cepellotti, A., Sabatini, R., Marzari, N., Kozinsky, B., AiiDA: automated interactive infrastructure and database for computational science. *Computational Materials Science.* **111**, 218–230, 10.1016/j.commatsci.2015.09.013 (2016).
[27] Schaarschmidt, J. *et al., Workflow* Engineering in Materials Design within the BATTERY 2030 + Project. *Advanced Energy Materials*, 2102638, 10.1002/aenm.202102638 (2021).
[28] Clark, S., Bleken, F.L., Friis, J., Anderson, C.W., Battery INterFace Ontology (BattINFO), BIG-MAP (2021).
[29] European Materials Modelling Council, EMMC, https://emmc.info/.

develop ontologies (e.g., EMMO), common knowledge-based representation systems, to ensure interoperability between multiple scales, different techniques and domains in the discovery process.

The development of the battery interface ontology BattINFO[30,31] was initiated within the BIG-MAP project and is being advanced in Battery 2030+. It is currently being integrated with other ontologies across different scales, such as manufacturing, to help battery experts in different fields translate real-life observations into a common digital representation. To lower adoption barriers and ensure broad uptake, several digital tools have been developed, including the BattINFO Converter.

Standardised infrastructures are now emerging that allow users to acquire, store, curate, and share data in consistent formats accessible from multiple platforms and for diverse purposes. A detailed and dynamic Data Management Plan (DMP) has been established to coordinate these efforts and ensure a linkage between data and tasks of the project[32]. To make it more operational, the DMP is being interconnected with BattINFO and, ultimately all the projects under the Battery 2030+ umbrella. It can possibly alter all EU battery projects, offering multiple layers of security and data-sharing, i.e., i) project-level, ii) Battery 2030+ restricted access, and iii) fully open source, e.g., in Materials Cloud (*https://www.marialscould.org*).

These efforts establish the semantic and digital foundation of the Battery 2030+ ecosystem, enabling seamless data exchange, accelerating innovation cycles, and positioning Europe at the forefront of global FAIR and ontology-driven materials research.

Multiscale modelling is essential to predict performance and lifetime. Battery performance and lifetime are determined by many processes on vastly different time and length scales[33]. Simulating batteries across scales from molecules to battery packs and beyond requires insight from very different time and length scales, following the EMMC guidelines: (1) *electronic scale*, allowing the description of chemical reactions – electronic density functional theory (DFT) and *ab initio* molecular dynamics (AIMD); (2) *atomistic and mesoscopic scale* – molecular dynamics (MD) and kinetic Monte Carlo (KMC) simulations; and (3) *macroscopic scale* continuum simulations[34].

A single differentiable computational model of virtual materials design encompassing all these phenomena and scales is beyond the limits of current computing power and theory. However, advances in ML models, and explainable AI (XAI) provide new possibilities for autonomous parameterisation and advanced/hierarchical multi-scaling[35]. Significant efforts have been made to coherently combine traditional single-scale models into multi-scale workflows[36], including the exploitation of AI and steps toward battery XAI. These methodologies have been made accessible to the community in the online app store and GitHub repository, *https://big-map.github.io/big-map-registry/*, where the protocols are shared. An overview of the potential impact of these techniques is given in Bhowmik *et al*.[37] multi-scale modelling techniques are currently being developed, for example,

[30] Clark, S., Bleken, F.L., Friis, J., Anderson, C.W., Battery INterFace Ontology (BattINFO), BIG-MAP (2021).
[31] Clark, S. *et al., Toward* a Unified Description of Battery Data. *Advanced Energy Materials.* **2021**, 2102702, 10.1002/aenm.202102702.
[32] Castelli, I.E., *et al., Data* Management Plans: The Importance of Data Management in the BIG-MAP Project (2021), https://arxiv.org/abs/2106.01616.
[33] Franco, A.A. *et al., Boosting* Rechargeable Batteries R&D by Multiscale Modeling: Myth or Reality? *Chemical Reviews.* **119** (7), 4569–4627, 10.1021/acs.chemrev.8b00239 (2019).
[34] Jeon, J., Yoon, G.H., Vegge, T., Chang, J.H., Phase-Field Investigation of Lithium Electrodeposition at Different Applied Overpotentials and Operating Temperatures. *ACS applied materials & interfaces.* **14** (13), 15275–15286, 10.1021/acsami.2c00900 (2022).
[35] Gunning, D. *et al., XAI*-Explainable artificial intelligence. *Science Robotics.* **4** (37), 10.1126/scirobotics. aay7120 (2019).
[36] Schaarschmidt, J. *et al., Workflow* Engineering in Materials Design within the BATTERY 2030 + Project. *Advanced Energy Materials*, 2102638, 10.1002/aenm.202102638 (2021).
[37] Bhowmik, A. *et al., Implications* of the BATTERY 2030+ AI-Assisted Toolkit on Future Low-TRL Battery Discoveries and Chemistries. *Advanced Energy Materials*, 2102698, 10.1002/aenm.202102698 (2021).

to optimise real and virtual electrode microstructures[38] and to study the effects of the fabrication process on cell performance[39] and electrode surface film growth.

Advanced characterisation across scales reveals the inner workings of batteries in unprecedented detail. Experimental characterisation of materials and interfaces is essential for mapping the chemical and structural space of batteries across time and length scales, from the atomic level to complete cells and systems. Multiple complementary datasets are required to capture cell behaviour, balancing fidelity (depth of understanding) and throughput (speed of screening).

Advanced characterisation at large-scale facilities such as synchrotrons and neutron sources[40]. provides data at unprecedented spatial and temporal resolution[41,42], including *operando* measurements in realistic cells. However, conventional characterisation often relies on isolated techniques, limiting the ability to correlate phenomena observed at different scales.

A large number of battery cell testing channels are being used for HT performance and aging evaluation for battery cells and systems. However, there is a clear need to go beyond the usual single-technique characterisation schemes and obtain a more holistic vision to connect the pieces of knowledge gained individually by stand-alone experiments[43]. This relies on new infrastructures, such as the European multimodal platform, initiated under BIG-MAP, that has embedded an array of ontologized tools capable of operating on request and producing multi-dimensional multi-parameter datasets.

Several facilities for combined data collection on batteries using multiple techniques simultaneously already exist, for example, European Synchrotron Radiation Facility (ESRF) beamline BM31, where X-ray absorption spectroscopy (XAS), X-ray diffraction (XRD) and total scattering (PDF) data can be collected quasi-simultaneously[44]. It calls for the ability to develop integrated and standardised multimodal workflows, including correlative analysis of multi-scale multi-technique data, and to perform autonomous, on-the-fly analysis of the vast amounts of data generated at laboratory, synchrotron, and neutron facilities across Europe.

In combination with big-data analytics using the advances in ML, multiplexing the heterogeneous sets of time-and-space-resolved data promises to enhance both the quality and quantity of meaningful observables. This approach provides multifaceted descriptions of reaction mechanisms across relevant scales under realistic conditions, at pertinent locations. The state of the art of the most relevant structural and spectroscopic characterisation techniques related to battery materials and interfaces is discussed in detail in Chapter 2.

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[38] Feinauer, J. *et al. MULTIBAT: Unified workflow for fast electrochemical 3D simulations of lithium-ion cells combining virtual stochastic microstructures, electrochemical degradation …* J. Comput. Sci. **31**, 172–184 (2019).
[39] Ngandjong, A.C. *et al.,* Multiscale Simulation Platform Linking Lithium-Ion Battery Electrode Fabrication Process with Performance at the Cell Level. *The journal of physical chemistry letters.* **8** (23), 5966–5972, 10.1021/acs.jpclett.7b02647 (2017).
[40] Black, A.P. *et al.,* Synchrotron radiation-based operando characterization of battery materials. *Chemical Science.* **14** (7), 1641–1665, 10.1039/d2sc04397a (2023).
[41] Sadd, M. *et al.,* Visualization of Dissolution-Precipitation Processes in Lithium–Sulfur Batteries. *Advanced Energy Materials.* **12** (10), 2103126, 10.1002/aenm.202103126 (2022).
[42] Graae, K.V. *et al.,* Time and space resolved operando synchrotron X-ray and Neutron diffraction study of NMC811/Si–Gr 5 Ah pouch cells. *Journal of Power Sources.* **570**, 232993, 10.1016/j.jpowsour.2023.232993 (2023).
[43] Atkins, D. *et al.,* Accelerating Battery Characterization Using Neutron and Synchrotron Techniques: Toward a Multi-Modal and Multi-Scale Standardized Experimental Workflow. *Advanced Energy Materials*, 2102694, 10.1002/aenm.202102694 (2021).
[44] Brennhagen, A. *et al*., (De)sodiation Mechanism of Bi2MoO6 in Na-Ion Batteries Probed by Quasi-Simultaneous Operando PDF and XAS. *Chemistry of Materials.* **36** (15), 7514-7524, 10.1021/acs.chemmater.4c01503 (2024).

Autonomous synthesis robotics,[45, 46] which can be controlled and directed by a central AI, is a central element of closed-loop materials discovery. Highly automated HT syntheses are now becoming state-of-the-art for organic and pharmaceutical research[47], and examples are also emerging in the development of solids and thin-film materials.[48,49] Automated HT synthesis of polymer electrolytes can draw considerable inspiration from well-established approaches for HT synthesis of organic molecules.

In contrast, automated HT synthesis of bulk inorganic materials is still in its early stages. For energy storage materials, robotic-assisted formulation[50], synthesis, manufacturing, and automation have opened the field to HT experimentation[51] with functional electrolytes and active materials for both positive and negative electrodes. However, introducing Li- or Na-ion battery materials, where structure and molecular vibration proxies, such as those involving transition metal ions, define the ion diffusion environment, presents broader challenges than those encountered in pharmaceuticals. Addressing these challenges requires a combined approach: developing both new methods and HT synthesis workflows that allow rapid fabrication and screening, while also leveraging ML- and AI-assisted algorithms to navigate large data sets.

Traditional synthesis routes for inorganic battery materials can be applied but are not always optimal for rapid screening. They require careful revision and evaluation against current technological capabilities to identify the best matches. Combined with computational approaches such as data mining and the correlation of structure–property relationships with the performance of battery active materials, automation has significantly impacted the discovery of novel and promising materials[52].

A key aspect is transforming from automation to autonomy in synthesis and characterization. Ideally, through the combined HT experimentation and computational approaches, one can significantly shorten the time spans from 10+ years per material in the battery field to gain a faster and more rapid integration. Another challenge is scaling up automation from the material level to the battery cell and system level, with robotics automating and accelerating performance and aging testing—an area currently being advanced within the FULL-MAP project.

Experimental and computational HT screening. Extensive libraries of compounds (e.g., salts, solvents, active materials, additives) can now be efficiently screened via the use of automated and miniaturised assays, which enable to accelerate of the electrode and electrolyte formulations R&D activities and optimised integration of relevant battery materials[53, 54]. Coupled with large-scale data analysis, acceleration of certain parts of the materials discovery process by up to one order of magnitude or

[45] Benayad, A. *et al.,* High-Throughput Experimentation and Computational Freeway Lanes for Accelerated Battery Electrolyte and Interface Development Research. *Advanced Energy Materials*, 2102678, 10.1002/aenm.202102678 (2021).
[46] Greenaway, R.L. *et al.,* High-throughput discovery of organic cages and catenanes using computational screening fused with robotic synthesis. *Nature communications.* **9** (1), 2849, 10.1038/s41467-018-05271-9 (2018).
[47] Wilkinson, M.D. *et al.,* The FAIR Guiding Principles for scientific data management and stewardship. *Scientific data.* **3**, 160018, 10.1038/sdata.2016.18 (2016).
[48] Benayad, A. *et al.,* High-Throughput Experimentation and Computational Freeway Lanes for Accelerated Battery Electrolyte and Interface Development Research. *Advanced Energy Materials*, 2102678, 10.1002/aenm.202102678 (2021).
[49] MacLeod, B.P. *et al.,* Self-driving laboratory for accelerated discovery of thin-film materials. *Science Advances.* **6** (20), eaaz8867, 10.1126/sciadv.aaz8867 (2020).
[50] Svaluto-Ferro, E. *et al.* Towards an Autonomous Robotic Battery Materials Research Platform Powered by Automated Workflow and Ontologized FAIR Data Management. Batteries & Supercaps, 10.1002/batt.202500155 (2025).
[51] Krishnamoorthy, A.N. et *al.,* Data-Driven Analysis of High-Throughput Experiments on Liquid Battery Electrolyte Formulations: Unraveling the Impact of Composition on Conductivity. Chemistry Methods, 10.1002/cmtd.202200008 (2022).
[52] Tabor, D.P. *et al.,* Accelerating the discovery of materials for clean energy in the era of smart automation. *Nature Reviews Materials.* **3** (5), 5–20, 10.1038/s41578-018-0005-z (2018).
[53] Benayad, A. *et al.,* High-Throughput Experimentation and Computational Freeway Lanes for Accelerated Battery Electrolyte and Interface Development Research. *Advanced Energy Materials*, 2102678, 10.1002/aenm.202102678 (2021).
[54] Schaarschmidt, J. *et al.,* Workflow Engineering in Materials Design within the BATTERY 2030 + Project. *Advanced Energy Materials*, 2102638, 10.1002/aenm.202102638 (2021).

more now can be achieved, although this still needs to be demonstrated for the full battery discovery process[55,56].

On the computational side, workflows have been developed to automate different steps of the calculations needed to screen for new compounds[57]. These workflows should be integrated with the HT experimentation with the computational feedback loops to drive adaptation and optimisation of the battery compounds in the HT experiments. Several examples of fully automated High-Throughput Experimentation (HTE) systems for electrolyte formulation, cell assembly, and selected relevant electrochemical measurements are now available[58].

AI in materials discovery offers excellent prospects[59], but the complexity and challenges of the autonomous discovery of novel battery materials and interfaces are at a much higher scale that can be handled by existing methods[60]. The availability of vast, curated datasets for training the models is a prerequisite for the successful application of AI/ML-based prediction techniques. Software packages such as ChemOS[61], Phoenics[62], Olympus[63], Hierarchical Experimental Laboratory Automation and Orchestration (HELAO)[64,65], FINALES[66] and Modular and Autonomous Data Analysis Platform (MADAP)[67] have been used in prototyping applications to demonstrate key components of an autonomous, self-driving laboratory, which has not yet been achieved for battery applications.

1.3 Challenges

Availability of FAIR and curated data

The development of predictive models to design future battery technologies requires thorough validation based on curated datasets with data of diverse quality (fidelity). In particular, the validation of the complex models required for the inverse design[68] of battery materials and interfaces requires the integration of high-fidelity data[69] covering complementary aspects of the material, interfacial and device characteristics. Currently, such datasets are sparse and cover only a fraction of the required data space; in particular, ontologies must be developed to make the data discoverable. The BIG-MAP Archive is one step closer to enabling this, however, it requires the battery community's increased engagement in sharing curated data.

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[55] Wildcat Discovery Technologies, http://www.wildcatdiscovery.com/#hs1.
[56] Chemspeed technologies, https://www.chemspeed.com/.
[57] Bölle, F.T., Bhowmik, A., Vegge, T., Maria García Lastra, J., Castelli, I.E., Automatic Migration Path Exploration for Multivalent Battery Cathodes using Geometrical Descriptors. *Batteries & Supercaps.* **4** (9), 1516–1524, 10.1002/batt.202100086 (2021).
[58] WWU Münster, Developing future super-batteries, https://www.uni-muenster.de/news/view.php?cmdid=10123&lang=en
[59] Stein, H.S., Gregoire, J.M., Progress and prospects for accelerating materials science with automated and autonomous workflows. *Chemical Science.* **10** (42), 9640–9649, 10.1039/C9SC03766G (2019).
[60] Lombardo, T. *et al.,* Artificial Intelligence Applied to Battery Research: Hype or Reality? *Chemical Reviews,* 10.1021/acs.chemrev.1c00108 (2021).
[61] Roch, L.M. *et al.,* ChemOS: Orchestrating autonomous experimentation. *Science Robotics.* **3** (19), 10.1126/scirobotics.aat5559 (2018).
[62] Häse, F., Roch, L.M., Kreisbeck, C., Aspuru-Guzik, A. ,Phoenics: A Bayesian Optimizer for Chemistry. ACS Central Science. 4 (9), 1134–1145, 10.1021/acscentsci.8b00307 (2018).
[63] Häse, F. et al. ,Olympus: a benchmarking framework for noisy optimization and experiment planning. Machine Learning: Science and Technology. 2 (3), 35021, 10.1088/2632-2153/abedc8 (2021).
[64] Hierarchical experimental laboratory automation and orchestration (HELAO) framework, https://github.com/helgestein/helao-pub.
[65] Rahmanian, F. et al. Enabling modular autonomous feedback-loops in materials science through hierarchical experimental laboratory automation and orchestration (2021).
[66] Vogler, M. et al. Brokering between tenants for an international materials acceleration platform (2022).
[67] Modular and Autonomous Data Analysis Platform (MADAP), https://github.com/fuzhanrahmanian/MADAP.
[68] Noh, J. *et al.,* Inverse Design of Solid-State Materials via a Continuous Representation. *Matter.* **1** (5), 1370–1384, 10.1016/j.matt.2019.08.017 (2019).
[69] Wilkinson, M.D. *et al.,* The FAIR Guiding Principles for scientific data management and stewardship. *Scientific data.* **3**, 160018, 10.1038/sdata.2016.18 (2016).

To accelerate development, a consolidated strategy to overcome current bottlenecks must be implemented to ensure the success of the Battery 2030+ initiative. Currently, the exploitability of existing data and databases remains very low, partly because of the vast size of the design space, and partly because system requirements impose constraints on materials that go beyond the optimisation of individual performance indicators. A central aspect is the uncertainty quantification and fidelity assessment of individual experimental and computational techniques as well as of generative deep learning, which pose a key challenge. Here, the central aspect is "knowing when you don't know" and knowing when additional data and training are needed[70] (see Figure 3).

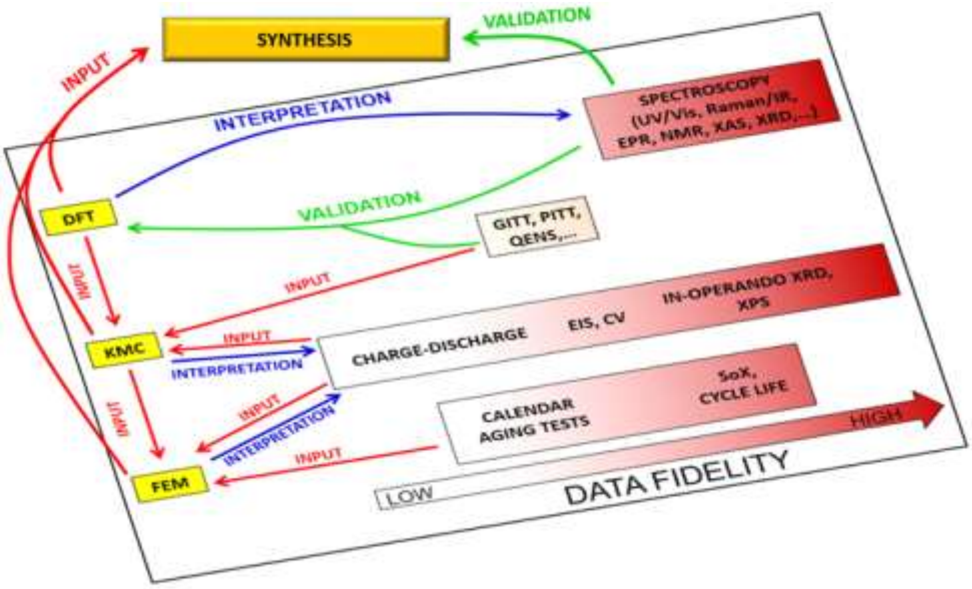

FIGURE 3. Illustration of the data flow between representative experimental and theoretical methods for studying battery interfaces. The fidelity of each method is generally proportional to its cost, but the fidelity–cost relationship can be optimised by acquiring data only when the given method/data is most valuable (adapted from[71]).

While ML has the potential to accelerate the screening and identification of, for example, structure–property relationships in inorganic energy materials[72], a key challenge in the discovery of battery materials and interfaces lies in developing autonomous workflows[73] capable of extracting fundamental relationships and knowledge from sparse datasets[74] that span a wide range of experimental and computational time and length scales.

In this context, connections to national efforts and consortia are of utmost importance. In Germany, the push for a national research data infrastructure has led to bespoke solutions in materials science, chemistry, and catalysis that are highly relevant to the battery field, such as NOMAD[75], NOMAD Oasis[76], and NOMAD Remote Tools Hub (NORTH)[77], which aim to integrate data management, instrument automation, and ML into a unified environment.

[70] Bhowmik, A. *et al.,* A perspective on inverse design of battery interphases using multi-scale modelling, experiments and generative deep learning. *Energy Storage Materials.* **21**, 446–456, 10.1016/j.ensm.2019.06.011 (2019).
[71] Ibid.
[72] Jennings, P.C., Lysgaard, S., Hummelshøj, J.S., Vegge, T., Bligaard, T., Genetic algorithms for computational materials discovery accelerated by machine learning. *npj Computational Materials.* **5** (1), 1–6, 10.1038/s41524-019-0181-4 (2019).
[73] Schaarschmidt, J. et al., Workflow Engineering in Materials Design within the BATTERY 2030 + Project. Advanced Energy Materials, 2102638, 10.1002/aenm.202102638 (2021
[74] Umehara, M. et al., Analyzing machine learning models to accelerate generation of fundamental materials insights. *npj Computational Materials.* **5** (1), 1–9, 10.1038/s41524-019-0172-5 (2019).
[75] https://nomad-lab.eu/nomad-lab/
[76] https://nomad-lab.eu/nomad-lab/nomad-oasis.html
[77] https://nomad-lab.eu/nomad-lab/nomad.html

Challenges for closed-loop materials discovery

To ensure the full integration of experimental and testing data into MAP, automated protocols for data acquisition and analysis must be developed. At present, there are few examples of automated robotics for solid-state synthesis[78] and automated cell assembly platforms. Complementary approaches and inspiration can be drawn from activities in related fields and consortia, such as the Canadian Acceleration Consortium (https://acceleration.utoronto.ca/) and the Danish Pioneer Centre for Accelerating P2X Materials Discovery (CAPeX, www.capex-p2x.com). Synthesis methods that have worked well to optimise battery materials in the lab may not always be the first line for HT and require careful evaluation.

Next to the automated HT synthesis, HT characterizations should be developed to validate the synthesized samples. This includes developing methodologies for the automated HT measurements (implementing robots, but in some cases adapting the sample preparation and measurement protocols to gain high efficiency). And then this requires developing tools for the automated analysis of the large amount of data generated. Two examples from the BIG-MAP project are the PRISMA and FullProfAPP, which enable automated phase analysis and Rietveld refinements of large sets of X-ray diffraction (XRD) data (large series of individual samples or operando XRD data). Such tools need to be developed for other characterizations techniques. Several ML–based tools have recently been developed to help in the data interpretation of relevant characterisation techniques, for example, NMR and XAS[79,80].

We also see a wide perspective to add here Raman spectroscopy as it is uniquely fit to capture light-weight elements like Li and Na and small structural changes in the realm defining diffusivity and capacity in those materials. These tools will enable automated analysis, but a wider portfolio of techniques with high predictability is needed to support a fully autonomous materials discovery platform. HT characterization could also be developed at large-scale facilities, as the advent of fourth-generation synchrotron and X-ray free electron lasers open perspectives towards serial screening of materials and devices, also permitted by the massive progress towards fast online data reduction and processing. The high brilliance and high coherence of nano/micro beams also enable them to observe the structure and dynamics of matter at unprecedented levels, promising discoveries at the particle and local interfaces scale and key high-precision information beyond the usual bulk averaged, or electrode averaged measures.

An important bottleneck in closed-loop discovery is the lack of robust and predictive models of key aspects of battery materials and concomitant interfaces. A key challenge in this regard is the urgent need to increase the predictive ability of material synthesizability by modelling (i.e., identifying suitable equilibrium and out-of-equilibrium computable descriptors that effectively control synthetic networks). This pertains both to physics/simulation-based and data-driven materials discovery strategies. Only the full integration of physics/simulation-based and data-driven models generated through the exploitation of AI technology and recent network science developments[81] with automated synthesis and characterisation technologies will enable the envisioned breakthroughs required for the implementation of fully autonomous materials discovery[82].

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[78] Seifrid, M. *et al. Routescore: Punching the Ticket to More Efficient Materials Development.* Cambridge University Press (CUP) (2021).
[79] Paruzzo, F.M. *et al.,* Chemical shifts in molecular solids by machine learning. *Nature Communications.* **9** (1), 4501, 10.1038/s41467-018-06972-x (2018).
[80] Suzuki, Y., Hino, H., Kotsugi, M., Ono, K., Automated estimation of materials parameter from X-ray absorption and electron energy-loss spectra with similarity measures. *npj Computational Materials.* **5** (1), 1–7, 10.1038/s41524-019-0176-1 (2019).
[81] Aziz, A., Carrasco, J., Towards Predictive Synthesis of Inorganic Materials Using Network Science. *Frontiers in chemistry.* **9**, 798838, 10.3389/fchem.2021.798838 (2021).
[82] Bhowmik, A. *et al.,* A perspective on inverse design of battery interphases using multi-scale modelling, experiments and generative deep learning. *Energy Storage Materials.* **21**, 446–456, 10.1016/j.ensm.2019.06.011 (2019).

Another aspect of closing the loop towards an accelerated materials discovery by automated data analysis is the broad implementation of ontologies and standards across all research areas which create input data for MAP.

In the short term, the development of an ontology defining a unified terminology and categories, properties, and relations for R&D data throughout Battery 2030+ is of high priority, with the BattINFO ontology and the BIG-MAP project's electronic lab notebook already in place[83,84]. The adoption of a unified ontology will be enabled and facilitated by implementing Electronic Lab Notebooks (ELNs). Ontologies and standards must eventually be made available by the scientific community. By their broad application, data will be made entirely FAIR. For one of the primary goals is to reach well-defined and standardised interfaces, enabling full reproducibility and interoperability. At this point, the Electronic Lab Notebook (ELN) could represent one step to the Platform as a Service (PaaS) and Lab as a Service (LaaS).

1.3.1 Advances needed to meet the challenges

The European research community is ready to support truly European effort dedicated to advancing our understanding of battery materials through the creation of a European Battery Materials Acceleration Platform. This initiative would build on examples of already existing initiatives at both multinational and national levels, such as ALISTORE-ERI[85], the French network for electrochemical energy storage and conversion devices (RS2E)[86], the Battery Pilot Hub in Grenoble[87], the Faraday Institution in the UK[88], and the Centre for Electrochemical Energy Storage Ulm & Karlsruhe (CELEST)[89], Münster Electrochemical Energy Technology (MEET)[90], Post Lithium Storage Cluster of Excellence (POLiS)[91] demonstrating that partnerships can be created beyond individual laboratories.

Autonomous synthesis and battery-cell characteristic test robotics

The complex nature of the material synthesis and electrochemical characterisation of battery cells and evaluation are among the major bottlenecks slowing the development of new battery materials and altering performances and stabilities for the batteries.[9,11] To explore larger classes of materials in the context of specific characteristics and optimisations of their structure-property relationships, it is essential to advance the development of HT synthesis robotics that address both electrolyte formulations and electrode active materials, alongside their combination, both for the characterisation of the materials as such and in the context of functional cells. This requires various approaches for synthesis methods starting from either precursor pre-screening and solution development up to solidified material/layer compounds of materials and cell-level characterisation of performance characterisation[92], as demonstrated by AutoBASS 1&2[93,94] Aurora, and other robotic platforms.

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[83] BIG-MAP, electronic lab notebook, big-map-notebook.eu.
[84] BIG-MAP, BattINFO ontology, https://github.com/BIG-MAP/BattINFO.
[85] https://i-mesc.eu/universite/alistore-eri
[86] https://www.energie-rs2e.com/en
[87] https://www.esrf.fr/HUB/PilotBattery
[88] https://www.faraday.ac.uk/
[89] https://www.celest.de/en/
[90] https://www.uni-muenster.de/MEET/en/institute/
[91] https://www.postlithiumstorage.org/en/
[92] Svensson, P.H. *et a.,* Robotised screening and characterisation for accelerated discovery of novel Lithium-ion battery electrolytes: Building a platform and proof of principle studies. Chemical Engineering Journal. **455**, 10.1016/j.cej.2022.140955 (2023)
[93] Zhang, B. *et al.,* Apples to apples: shift from mass ratio to additive molecules per electrode area to optimize Li-ion batteries. Digital Discovery, **3**, 1342-1349, *10.1039/D4DD00002A* (2024)
[94] Zhang, B. *et al.,* Robotic cell assembly to accelerate battery research. Digital Discovery, **1**, 755-762, *10.1039/D2DD00046F* (2022)

High-throughput/high-fidelity characterisation

While an increasing number of approaches for HT evaluation of battery materials are reported in the literature,[95,96] many electrochemical tests remain time-intensive; for example, cycling experiments can take days, months, or even years[97]. To fully exploit the potential of testing large numbers of samples, and ensure reproducibility of results, an automated HT infrastructure for *in situ* and *operando* characterization of battery materials and cells must be established. This includes the development of versatile multimodal cells, standardized galvanostatic cycling protocols, and efficient sample transfer methods. The infrastructure should address both breadth and depth, incorporating filtration steps to focus on identified hit/lead candidates.

A critical factor influencing battery kinetics and thermodynamics is the microstructure and defects in the electrodes; these should be considered when fine-tuning electrode design. Tailoring these aspects requires greater emphasis on multiscale microstructural characterization of electrodes and solid-state electrolytes for next-generation batteries[98]. Combining physics-guided, data-driven modelling with systematic data generation will be key to enabling HT battery testing. Such integration will accelerate the discovery of new materials and interfaces by embedding them directly into active material development workflows.

A cross-sectoral data infrastructure

Accelerated materials innovation relies on the appropriate and shared representation of both data and the physical and chemical insights obtained from them[99,100]. This poses a substantial challenge to the international research community, which needs to join forces in establishing, populating, and maintaining a shared materials data infrastructure as well as corresponding data interfaces and standards. Establishing a common data infrastructure will help ensure the interoperability and integration of experimental data and modelling in a closed-loop materials discovery process across institutions in real time. Realising such an infrastructure will make the data generated by individual groups and consortia instantly available to the community at large and drastically shorten R&I cycles. MAP will pioneer such an infrastructure based on a decentralised access model in which data, simulation protocols, and AI-based discovery tools and components from different sources can be used *via* qualified access protocols.

Scale bridging and integrated workflows[101,102]

The root of the multi-scale challenge lies in the fact that it is not yet clear how to effectively and robustly couple models and correlative data analysis across different scales. Essentially, all effects

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[95] Hahn, R. *et al.,* High-throughput battery materials testing based on test cell arrays and dispense/jet printed electrodes. *Microsystem Technologies.* **25** (4), 1137–1149, 10.1007/s00542-019-04368-5 (2019).

[96] Lyu, Y., Liu, Y., Cheng, T., Guo, B., High-throughput characterization methods for lithium batteries. *Journal of Materiomics.* **3** (3), 221–229, 10.1016/j.jmat.2017.08.001 (2017).

[97] Harlow, J.E. *et al.,* A Wide Range of Testing Results on an Excellent Lithium-Ion Cell Chemistry to be used as Benchmarks for New Battery Technologies. *Journal of The Electrochemical Society.* **166** (13), A3031-A3044, 10.1149/2.0981913jes (2019).

[98] K. Daems et al., Advances in inorganic, polymer and composite electrolytes: Mechanisms of Lithium-ion transport and pathways to enhanced performance. *Renewable and Sustainable Energy Reviews*, **191**, 114136, ISSN 1364-0321, 10.1016/j.rser.2023.114136 (2024).

[99] Greenaway, R.L. et al., High-throughput discovery of organic cages and catenanes using computational screening fused with robotic synthesis. *Nature communications.* **9** (1), 2849, 10.1038/s41467-018-05271-9 (2018).

[100] Bai, Y. *et al.,* Accelerated Discovery of Organic Polymer Photocatalysts for Hydrogen Evolution from Water through the Integration of Experiment and Theory. *Journal of the American Chemical Society.* **141** (22), 9063–9071, 10.1021/jacs.9b03591 (2019).

[101] Atkins, D. *et al.,* Accelerating Battery Characterization Using Neutron and Synchrotron Techniques: Toward a Multi-Modal and Multi-Scale Standardized Experimental Workflow. *Advanced Energy Materials*, 2102694, 10.1002/aenm.202102694 (2021).

[102] Schaarschmidt, J. *et al.,* Workflow Engineering in Materials Design within the BATTERY 2030 + Project. *Advanced Energy Materials*, 2102638, 10.1002/aenm.202102638 (2021).

observed at the macroscopic level (e.g., in a cell) originate from phenomena at the atomistic level, which are generally quantum in nature. The large gains in accessible time scales and system sizes offered by larger-scale models typically come at the cost of detail and resolution. While substantial progress has been made in specific use cases for multiscale method development, unlocking the full potential of multi-scale experimental characterization, modelling, and inverse design requires sustained, coordinated efforts from both the modelling and experimental communities. Integrated approaches that connect scales beyond the current state of the art are needed to tackle open challenges such as state-of-health (SoH), manufacturability, and the sustainability of batteries.[103] This can be achieved only by establishing interoperable workflows that can communicate across various workflow engines, simulation codes, and experiments.

ML techniques and other physics-guided, data-driven models can identify the most important parameters, features, and fingerprints[104], as well as bridge scales where no clear model overlap exists. They can also guide experiment design, and the analysis of multiple datasets collected across extended time and length scales, going beyond standard single-shot, stand-alone experiments. Where no physical models are available, surrogate models can be employed. There is great potential to codify workflows so they can be used outside the developing group via accessible app-stores. In addition to purely computational workflows, those integrating on-the-fly or highly specific cutting-edge experiments (and vice versa) hold great promise for accelerating materials discovery. The integrated technologies enabling such workflows are just becoming accessible.

MAP will leverage European computational infrastructures, such as those offered by PRACE and European High Performance Computing Joint Understanding[105] (EuroHPC JU)'s European AI factories, as well as outcomes from prior and ongoing EU and national initiatives, including former and current HPC centres of excellence such as NOMAD and MaX. MAP will also draw on European experimental platforms, such as the European Battery Hub, which provide new access modes to synchrotron and neutron facilities and offer a collaborative framework for AI-aided, standardized multimodal characterisation. While most current simulation and experimental efforts focus on understanding battery function, with increasing emphasis on design, additional work is needed to develop models that address the full battery life cycle.

AI exploitation

AI-based generative models[106], i.e., probabilistic models that capture the spatio–temporal evolution of battery materials and interfaces, can significantly contribute to the objectives of the MAP. Developing hybrid models that combine physics and data-driven approaches will be an essential component of this effort.

Currently, there are significant gaps in the spectrum of battery models, which preclude the development of comprehensive and accurate representations. Although AI-based techniques can potentially address these gaps, they often lack awareness of physical laws, leading to potential violations. The key to overcoming this dilemma is the development of hybrid models, which incorporate both AI-based predictions and the constraints imposed by the laws of physics. By combining the strengths of AI and physical models, we can create a synergy wherein AI is employed to adapt and enhance physical models or where the laws of physics appropriately bind the prediction space of AI-based models. However, these models must be trained on large, curated datasets from advanced multi-scale computational modelling, materials databases, the literature[153], and *operando*

[103] Noh, J. *et al.,* Inverse Design of Solid-State Materials via a Continuous Representation. *Matter.* **1** (5), 1370–1384, 10.1016/j.matt.2019.08.017 (2019).
[104] Reichstein, M. *et al.,* Deep learning and process understanding for data-driven Earth system science. *Nature.* **566** (7743), 195–204, 10.1038/s41586-019-0912-1 (2019).
[105] https://www.eurohpc-ju.europa.eu/index_en
[106] Noé, F., Olsson, S., Köhler, J., Wu, H., Boltzmann generators: Sampling equilibrium states of many-body systems with deep learning. *Science.* **365** (6457), 10.1126/science.aaw1147 (2019).

characterisation. These data must span all aspects of battery materials from synthesis to cell-level testing[107].

Unification of protocols[108,109]

MAP will offer a unique opportunity to leverage the size of this effort in the interest of standardising data and workflow methodologies from the entire battery value chain, by exploiting semantic access protocols enabled by EMMC and EMMO and by tapping private groups, with the goal of connecting academia and industry, materials modelling and engineering[110]. The development of an **Open Battery Innovation Platform** is needed to facilitate the sharing of infrastructures and data between partners and the integration of modelling into industrial processes to close the gap between *in silico* materials design, battery cell manufacturing, and their end use in everyday devices.

The inverse design of battery materials and interfaces effectively inverts the traditional discovery process by allowing the desired performance goals to define the composition and structure of the battery materials and/or interfaces that best meet the targets without a priori defining the starting materials.

1.4 Forward Vision

We are developing a versatile, chemistry-neutral framework aimed at achieving a 5–10× acceleration in the discovery of novel battery materials and interfaces. This effort is now being extended and intensified through the FULL–MAP project (2025–2029), which will reshape the European battery research and innovation landscape. It will reinvent the entire battery materials and interfaces discovery value chain by combining AI–guided robotic synthesis, autonomous HT and operando characterization, smart cell assembly, predictive digital twins, and adaptive performance evaluation. Together, these capabilities will usher in a new era of self-driving laboratories and a fully integrated, intelligent discovery ecosystem—unprecedented in battery science.

In the short-term (2025–2027): To establish modular, chemistry-agnostic MAP prototypes within participating laboratories, enabling broad applicability across diverse research environments. A key objective is to validate autonomous, closed-loop workflows in multiple experimental use cases, demonstrating the platform's flexibility and robustness. To ensure seamless semantic data flow, tools such as PerQueue[111] and BattINFO will be integrated into practical lab operations. In parallel, joint benchmarking activities will be launched to assess and compare MAP efficiency across laboratories. AI tools will be trained to support experiment planning, error detection, and early-stage screening—laying the groundwork for smarter and faster discovery cycles.

In the medium-term (2027–2030): To achieve robust interoperability between distributed MAP nodes across Europe, enabling seamless collaboration and shared progress, by optimizing AI-assisted workflows to accelerate iteration cycles and refine scientific hypotheses. The platform will expand to address poorly understood materials, interfaces, and microstructural phenomena, targeting key knowledge gaps in emerging battery chemistries. At the technical level, standardized Application Programming Interfaces (APIs) and ontologies will be developed to facilitate plug-and-play integration of new tools and technologies. MAP discovery workflows will increasingly couple with simulation

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[107] Bhowmik, A. *et al.,* A perspective on inverse design of battery interphases using multi-scale modelling, experiments and generative deep learning. *Energy Storage Materials.* **21**, 446–456, 10.1016/j.ensm.2019.06.011 (2019).

[108] Schaarschmidt, J. *et al.,* Workflow Engineering in Materials Design within the BATTERY 2030 + Project. *Advanced Energy Materials*, 2102638, 10.1002/aenm.202102638 (2021).

[109] Sjølin, B.H. *et al.,* Accelerated Workflow for Antiperovskite-based Solid State Electrolytes. *Batteries & Supercaps.* **6** (6), 10.1002/batt.202300041 (2023).

[110] Goldbeck Consulting, Materials Modelling - Connecting communities: science to engineering, academia to industry, https://materialsmodelling.com/.

[111] Simon K. Steensen, et al., The Necessity of Dynamic Workflow Managers for Advancing Self-Driving Labs and Optimizers, Advanced *Intelligent Discovery,* 202500067, (2025).

inputs and scale-up constraints, such as processability and recyclability, to ensure alignment with real-world manufacturing and sustainability goals.

In the long-term (2030 and beyond): The ambition is to realize a 5-10x acceleration in the discovery and validation of sustainable battery materials. This will involve deploying fully autonomous MAPs capable of operating with minimal human intervention. A Europe-wide network of MAP nodes will be established to share protocols, data, and experimental capabilities—fostering collaboration and maximizing impact. Crucially, closed data loops will connect early-stage discovery to battery design, production, and end-of-life systems, ensuring a holistic and efficient innovation cycle.

Accelerated Materials Discovery represents a central methodology in battery research. While foundational concepts and tools have been defined, full implementation remains a work in progress and will require continued investment and coordination. The next phase of the BATTERY 2030+ Roadmap should focus on scaling and generalizing the MAP concept, embedding semantic standards, and linking discovery workflows to the broader battery value chain. The potential rewards are significant: faster innovation, deeper scientific insight, and a more sustainable, resilient, and competitive European battery ecosystem.

2. BATTERY INTERFACE GENOME (BIG)

Interfaces and interphases remain one of the most critical bottlenecks in the development of high-performance, safe, and durable batteries — particularly for next-generation systems such as solid-state, sodium-based batteries or multivalent chemistry families. Despite significant progress in recent years, the dynamic and complex nature of these interfaces continues to pose major challenges for both characterization and predictive design.

Interfaces in batteries are arguably the least understood aspect of these systems, even though most critical battery reactions - such as charge transfer, dendrite formation, solid electrolyte interphase (SEI) and cathode electrolyte interface (CEI) formation – occur there. Building on the foundation laid by BIG-MAP (2020-2024), Battery 2030+ has proposed the development of the Batteries Interface Genome (BIG)[112], which aims to establish a new basis for understanding the interfacial processes that govern the operation and performance of every battery.

Three Battery 2030+ projects are at the core of this research area: **OPERA**, **OPINCHARGE**, and **ULTRABAT**. Together, they aim to provide a multiscale understanding of interface phenomena, combining operando experiments with atomistic and continuum simulations. OPERA brings in the development of *operando* techniques and multiscale modelling to face the zero-excess solid state battery challenge. OPINCHARGE brings in multi-physics modelling of interface dynamics, particularly for solid electrolyte interphase (SEI) formation, characterisation and silicon voltage hysteresis, ULTRABAT adds an understanding of ultrafast transport processes in cathode materials, such as LMO, as well as across the SEI, from atomistic simulations to synchrotron experiments.

Several key priorities have emerged for advancing the understanding and control of battery interfaces. First, *operando* tools must be adapted to real-world relevance, meaning high-resolution characterisation techniques should be applied to analysing interfaces within fully operating cells.

Second, reliability, reproducibility, and representativeness of *operando* studies, including the possible impact of the probe radiation on the sample and its electrochemistry[113]. Research efforts should also prioritize sodium-ion and solid-state battery systems, where interfacial stability issues remain poorly understood yet have a critical impact on lifetime and safety. To ensure comparability and accelerate progress, there is a growing need for the standardization of interface metrics, defining clear criteria for what constitutes a "good" interface in terms of resistance, stability, morphology, and reactivity across different battery chemistries.

2.1 Introduction

Experience has shown that when developing new battery chemistries or introducing new functionalities into existing battery technologies, interfaces hold the key to unlocking the full potential of electrode and electrolyte materials, enabling the creation of ultra-high-performance, sustainable, and smart batteries. The European battery R&D landscape comprises numerous leading research institutions, laboratories, and industries, many pursuing complementary approaches to this challenge

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[112] Atkins, D. *et al.,* Accelerating Battery Characterization Using Neutron and Synchrotron Techniques: Toward a Multi-Modal and Multi-Scale Standardized Experimental Workflow. *Advanced Energy Materials*, 2102694, 10.1002/aenm.202102694 (2021).

[113] Drnec, J., Lyonnard, S., Battery research needs more reliable, representative and reproducible synchrotron characterizations, *Nature Nanotechnology* **20**(5), 584-587, 10.1038/s41565-025-01921-4 (2025).

in isolation. With the BIG, we aim to unite expertise across sectors, industries, and end users to accelerate the development and deployment of radically new battery technologies.

Existing research methodologies largely rely on incremental advances at the local scale, which are insufficient to tackle the ambitious challenges within the timeline outlined in this Roadmap. Thus, the MAP will provide the infrastructural backbone to accelerate the application of new findings, while BIG will continue to develop the necessary understanding and models to predict and control the formation and dynamics of crucial interfaces and interphases that limit battery performance and safety[114].

The ongoing research under the Battery 2030+ initiative ensures that BIG remains highly adaptive to different chemistries, materials, and designs. This includes technologies beyond the current state-of-the-art lithium-ion systems, where substantial data and insights exist for model training, as well as emerging technologies such as sodium-ion, all-solid-state, and radically new chemistries.

Batteries comprise not only an interface between the electrode and the electrolyte but a number of other important interfaces, for example, between the current collector and the electrode and between the active material and the additives, such as conductive carbon and/or binder and buried interfaces. Important also are interfaces between several types of active materials in composites and/or complex nanostructures with a hierarchy of active particles. Realising this, any globally leading approach to mastering and inversely designing battery interfaces must combine the characterisation of these interfaces in time as well as in space (i.e., spatio–temporal characterisation) with hybrid physical- and uncertainty-aware data-driven models[115,116]. Thereby integrating dynamic events at multiple scales, e.g., across the atomic and micrometer scales. In this respect, we must consider studies of ion transport mechanisms through interfaces and, even more challenging, visualise the role of the electron in these interfacial reactions. When mastered, interfacial reactivity helps to extend the thermodynamic and kinetic stability of organic electrolytes used in batteries; when it is not controlled, however, continuous parasitic reactions may occur, limiting the cycle life of batteries. The complexity of such interphases arises from multiple reactions and processes spanning a wide range of time and length scales that define their formation, structure, dynamics and, ultimately, their functionality in the battery. Their structural properties depend in a highly complex and elusive manner on the specific characteristics of the composition of the electrolyte, the structures of the electrode materials, and the external conditions. Understanding, controlling, and designing the function of interfaces and interphases[117] is, therefore, key for the development of ultra-performing, smart, and sustainable batteries.

The BIG can be related to the concept of descriptors in catalyst design[118], in which the binding energy of important reaction intermediates scales with that of the descriptor, and the identification and quantification of the descriptor value enables an accelerated and accurate prediction of the rate of the total reaction. Identifying the multiple dynamic descriptors (or genes) coding for the spatio–temporal evolution of battery interfaces and interphases is a prerequisite for the inverse design process and simply cannot be done using existing, individual methodologies, but requires multimodal insight and

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[114] Diddens, D. *et al.,* Modeling the Solid Electrolyte Interphase: Machine Learning as a Game Changer? *Advanced Materials Interfaces*, 2101734, 10.1002/admi.202101734 (2022).
[115] Busk, J. *et al.,* Calibrated uncertainty for molecular property prediction using ensembles of message passing neural networks. *Machine Learning: Science and Technology.* **3** (1), 15012, 10.1088/2632-2153/ac3eb3 (2022).
[116] Busk, J., Schmidt, M.N., Winther, O., Vegge, T., Jørgensen, P.B. *Graph Neural Network Interatomic Potential Ensembles with Calibrated Aleatoric and Epistemic Uncertainty on Energy and Forces* (2023).
[117] Atkins, D. *et al.,* Accelerating Battery Characterization Using Neutron and Synchrotron Techniques: Toward a Multi-Modal and Multi-Scale Standardized Experimental Workflow. *Advanced Energy Materials*, 2102694, 10.1002/aenm.202102694 (2021).
[118] Nørskov, J.K., Bligaard, T., The catalyst genome. *Angewandte Chemie International Edition.* **52** (3), 776–777, 10.1002/anie.201208487 (2013).

machine-learning-based approaches to unfold.[119,120,121] This requires improving the capabilities of multi-scale modelling, machine- and deep learning, and systematic multi-technique characterisation of battery interfaces, including *operando* characterisation, to generate/collect comprehensive sets of high-fidelity data[122,123] that will feed a common AI-orchestrated data infrastructure in MAP. BIG aims at establishing the fundamental “genomic” knowledge of battery interfaces and interphases through time, space, and chemistries. The BIG will be chemistry neutral, starting from state-of-the-art Li-ion technology, where substantial data and insights are available for training the models, to emerging technologies like Na-ion and all-solid-state and radically new chemistries.

2.2 Current Status

Battery interfaces and interphases – where the energy storage in batteries is facilitated but also where many degradation phenomena are initiated, have always been both a blessing and a major limitation in battery development. For instance, the growth of the SEI on the anode as well as cathode electrolyte interphase (CEI) on the cathode has both a significant impact on the one galvanostatic cycling stability as well as safety of LIBs. Thus, when mastered, interfacial reactivity helps to extend the thermodynamic and kinetic stability of organic electrolytes used in batteries; when it is not controlled, however, continuous parasitic reactions may occur, limiting the cycle life of batteries.[124] Understanding, controlling, and designing the function of interfaces and interphases is, therefore, key for the development of ultra-performing, smart, and sustainable batteries.

In comparison with the bulk dimensions of the electrode and electrolyte (~µm), the interface (or interphase) is several orders of magnitude smaller (~nm), and interfacial reactions are easily masked by their surroundings. Experimental and computational techniques must therefore be highly surface sensitive with exceptionally high resolution to probe such buried interfaces. Nevertheless, the experimental characterisation of battery interfaces has been an enduring challenge. Indeed, very few, if any, techniques can provide a full description of the events happening at the electrode-electrolyte interface.

Thus, no singular technique is currently capable of providing a comprehensive description of events happening at the many types of buried interfaces. This opens significant opportunities to support experiments with high-fidelity computational and machine learning models, in parallel to the development of characterisation techniques capable of probing the chemical and morphological properties of interphases, intensive research efforts have been devoted to developing chemical and engineering approaches to control the dynamics of the interphases upon galvanostatic cycling. The most prominent approach is using electrolyte additives/co-solvents that react inside the cell during initial operation and coatings that can passivate the surface of electrode materials and thus prevent inevitable reactivity with the electrolyte. However, many years of Edisonian trial-and-error research have demonstrated the need to use several functional additives working in synergy to achieve an effective electrode-electrolyte interface. Accelerated development of such an interphase would

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[119] Bhowmik, A., Castelli, I.E., Garcia-Lastra, J.M., Jørgensen, P.B., Winther, O., Vegge, T., A perspective on inverse design of battery interphases using multi-scale modelling, experiments and generative deep learning. *Energy Storage Materials.* **21**, 446, 10.1016/j.ensm.2019.06.011 (2019).

[120] Rieger, L.H., Cadiou, F., Jacquet, Q., Vanpeene, V., Villanova, J., Lyonnard, S., Vegge, T., Bhowmik, A., Utilizing active learning to accelerate segmentation of microstructures with tiny annotation budgets, *Energy Storage Materials*. **73**, 103785 (2024).

[121] Han, S., Lysgaard, S., Vegge, T., Hansen., H. A. Rapid mapping of alloy surface phase diagrams via Bayesian evolutionary multitasking. *npj Computational Materials* **9**, 139 (2023).

[122] Schreiner, M., Bhowmik, A., Vegge, T., Busk, J., Winther, O., Transition1x - a dataset for building generalizable reactive machine learning potentials. *Scientific Data.* **9** (1), 779, 10.1038/s41597-022-01870-w (2022).

[123] Schreiner, M., Bhowmik, A., Vegge, T., Jørgensen, P.B., Winther, O., NeuralNEB—neural networks can find reaction paths fast. *Machine Learning: Science and Technology.* **3** (4), 45022, 10.1088/2632-2153/aca23e (2022).

[124] Appiah, W. A.,Rieger, L. H., Flores, E., Tejs Vegge, T., Bhowmik, A., Unravelling degradation mechanisms and overpotential sources in aged and non-aged batteries: A non-invasive diagnosis. *J. Energy Storage*. **84**, 111000 (2024)

greatly benefit from HT techniques and AI-assisted rationalisation. We see perspective in defining such model fast screen interphase systems for stability and diffusion studies by using thin and thick film tech and other methods for fast alterations of the interphase microstructure and chemistry. In fast screen diagnostics, methods looking at the interphase based on spectroscopy are ideal for differentiating through frequency tailoring and possibly wavelength screening close and far from the interphase changes in chemistry and structures.

Physics- and uncertainty-aware data-driven methods

The complexity of electrochemical systems usually motivates the simplification of simulations such that they only qualitatively mimic the real situation in the battery or the experiment. A coupling of physics-aware data-driven methods would strongly enhance the quality of the determination of interface descriptors, features, and parameters by enriching the physical simulation with validated correlations between idealised physics/chemistry-based simulations and data on real materials. Interoperability and scale-coupling are also a challenge for experiments, requiring non-intrusive *operando* data acquisition on realistic cells working in representative conditions and subsequent AI-aided correlative analysis of large data sets.

A complete and closed mathematical description of the whole reaction mechanism is enormously challenging and unlikely comprehensible, since coupled ionic and electronic transfer reactions in an electrochemically relevant environment usually include coupled multistep reactions[125,126]. These multistep reactions are often either oversimplified or the reaction steps are modelled in too ideal environments[127]. In specific cases, it is possible to combine Density Functional Theory (DFT) methods with classical approaches to improve the description of surface reactions[128], but generic approaches remain limited, and an efficient and systematic coupling is still lacking.

2.3 Challenges

Interfaces and Interphases

Despite decades of research, the details of interfacial reactions in the complex electrochemical environments in batteries (e.g., the composition and function of the SEI) remain mysteries. The structural properties depend in a highly complex and elusive manner on the relevant properties of the electrolyte components and resulting compositions, the structures of the electrode materials, and the external conditions. The complexity of such interphases arises from multiple reactions and processes spanning a wide range of time and length scales that define their formation, structure, and, ultimately, their functionality in the battery.

Intensive efforts were made in recent years to uncover the complexity of the interface dynamics and to control its reactivity and functionality, acquiring an enormous dataset whose depth remains largely under-exploited. Data must be collected, handled, and analysed in a systematic and automated/autonomous manner to be accessible to the central BIG-MAP AI, orchestrating the accelerated discovery process[129].To ensure meaningful synergy between experiments, simulations, and AI-based models, simulations and models need to become more realistic and include experimental

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[125] Bruce, P.G., Saidi, M.Y., The mechanism of electrointercalation. *Journal of Electroanalytical Chemistry.* **322** (1-2), 93–105, 10.1016/0022-0728(92)80069-g (1992).

[126] Lück, J., Latz, A., Modeling of the electrochemical double layer and its impact on intercalation reactions. *Physical chemistry chemical physics: PCCP.* **20** (44), 27804–27821, 10.1039/C8CP05113E (2018).

[127] van Duin, A.C.T., Dasgupta, S., Lorant, F., Goddard, W.A., ReaxFF: A Reactive Force Field for Hydrocarbons. *The Journal of Physical Chemistry A.* **105** (41), 9396–9409, 10.1021/jp004368u (2001).

[128] Eberle, D., Horstmann, B., Oxygen Reduction on Pt (111) in Aqueous Electrolyte: Elementary Kinetic Modeling. *Electrochimica Acta.* **137**, 714–720, 10.1016/j.electacta.2014.05.144 (2014).

[129] Stier, *et al.,* Materials Acceleration Platforms (MAPs): Accelerating Materials Research and Development to Meet Urgent Societal Challenges. *Advanced Materials.* 10.1002/adma.202407791 (2024).

conditions. Similarly, the experimental conditions should be as reproducible and exact (i.e., ideal) to decouple effects and reactions.

Multi-scale modelling concepts: Key challenges in this regard include the development of new multi-scale modelling concepts (including physics-aware data-driven hybrid models to identify interphase descriptors) and the development of new characterization techniques, particularly under electrochemical conditions relevant to the application. Datasets enabling the training of such models are just becoming available now. Standardisation of experimental data, conditions, and observables as inputs to physical models to make the link between observables and descriptors.

A fundamental understanding is the first step in controlling the complex and dynamic processes at the interfaces in emerging high-performance battery technologies. This understanding relies on the availability and development of adequate experimental and computational tools capable of probing the evolution of the dynamic processes occurring at the battery interfaces and making them understandable to scientists. These tools should selectively provide information on the interface region, and special efforts must be made to couple complementary experimental, simulation-based, and AI-based modelling tools[130]. It could be envisioned that mature battery interface/interphase characterisation techniques could provide HT experimental input about battery interfaces during operation. One of the key challenges in establishing BIG is to automate the acquisition, curation, and analysis of large datasets. These could feed the physics-aware data-driven hybrid models that will help better understand and predict interfacial properties and enable direct multi-scale bridging by developing integrated multimodal workflows for correlative characterization.

Combining physical and data-driven models

This will only be possible if datasets are acquired from reliable temporally and spatially resolved experiments, including data recorded under working conditions (i.e., *operando* measurements) and spanning the full range from optimised laboratory-based to large-scale research-facility–based measurements and HT synthesis and laboratory testing. Combining physical and data-driven models run on curated community-wide datasets spanning multiple domains in the discovery process will enable us to establish the BIG[131,132] for interphase development and dynamics. This has the potential to lay the foundation for the inverse design of battery interfaces/interphases[133] for example, using region-based active learning algorithms[134,135].

Uncertainty quantification

Understanding and tracking different types of uncertainties in the experimental and simulation methods, as well as in the machine learning framework of, for example, unsupervised[136] and

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[130] Steinrück, H.-G. *et al.,* Correction: The nanoscale structure of the electrolyte–metal oxide interface. *Energy & Environmental Science.* **11** (4), 996, 10.1039/c8ee90018c (2018).
[131] Radford, A., Metz, L., Chintala, S. *Unsupervised Representation Learning with Deep Convolutional Generative Adversarial Networks.* 4th International Conference on Learning Representations, ICLR 2016 - Conference Track Proceedings 1–16 (2016).
[132] Ceriotti, M., Unsupervised machine learning in atomistic simulations, between predictions and understanding. *The Journal of Chemical Physics.* **150** (15), 150901, 10.1063/1.5091842 (2019).
[133] Bhowmik, A. *et al.,* A perspective on inverse design of battery interphases using multi-scale modelling, experiments and generative deep learning. *Energy Storage Materials.* **21**, 446–456, 10.1016/j.ensm.2019.06.011 (2019).
[134] Nørskov, J.K., Bligaard, T., The catalyst genome. *Angewandte Chemie International Edition.* **52** (3), 776–777, 10.1002/anie.201208487 (2013).
[135] Cortes, C., DeSalvo, G., Gentile, C., Mohri, M., Zhang, T., Region-Based Active Learning. *Proceedings of the Twenty-Second International Conference on Artificial Intelligence and Statistics, PMLR,* 89:2801-2809 (2019).
[136] Radford, A., Metz, L., Chintala, S. *Unsupervised Representation Learning with Deep Convolutional Generative Adversarial Networks.* 4th International Conference on Learning Representations, ICLR 2016 - Conference Track Proceedings 1–16 (2016).

generative deep learning models[137], is crucial for controlling and improving the fidelity of the predictive design of interphases. Simultaneous utilisation of data from multiple domains, including data from an apparently failed experiment[138], can accelerate the development of generative models that enable the accelerated discovery and inverse design of durable high-performance interfaces and interphases in future batteries. The ESRF, for example, is releasing all its experimental data, but only for the structural results, so unless the corresponding electrochemical data can be found, the *operando* data is of limited use.

2.3.1 Advances needed to meet the challenges

Novel computational and experimental techniques and their combination

The development of new computational and experimental techniques targeting increased spatial resolution, time domains, and *operando* conditions is needed to generate new insights into the construction of ultra-high-performing battery systems. Realising this development is challenging for both theoretical and experimental science, and enhanced collaboration between disciplines is necessary to unlock the next generation of battery technologies. Experimental input is needed to identify realistic input parameters for the development of new computational models, and modelling results need to be validated against experimental results[139]. Likewise, the interpretation of experimental results can be made with higher precision if theoretical models can be used in combination with experiments.

High-quality, high-fidelity data and insights are essential for developing the BIG. This necessitates the advancement of superior *operando* experimental techniques to establish atomic-level understanding across various spatial and temporal scales. Moreover, real-time acquisition and analysis should be targeted to provide instantaneous input for the materials acceleration platform developed within MAP. Consequently, BIG offers a unique opportunity to establish a common European platform and harmonized battery standards for data acquisition and transfer, which could play the role of a key demonstrator in new large-scale European initiatives like the Materials Commons[140].

In addition to the continuous improvement of optimised existing as well as development of new experimental techniques and methodologies targeting the scale of atoms and ions and spatially resolving heterogeneous distributions of atoms and ions from nano to meso and micro-scales, radically new ways of combining experimental, theoretical, and data-driven techniques will be necessary. For example, developing novel experimental and computational techniques targeting the time and length scales of electron localisation, mobility, transfer reactions, ion dynamics, and distributions. Advanced physics-based hybrid models and simulation techniques must be used for the interpretation of cutting-edge operando experiments. Efficient methods for using large datasets to determine the descriptors of multi-scale/multi-structure theories must be developed. This should also include recent progress on graph and network theory applied to electrolyte interphase formation[141]. With these technical advances, new insights will follow, allowing us to control access to the fine-tuning of the battery interface and thus develop the next generation of ultra-high-performing batteries.

Standardised testing protocols and interoperability

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[137] Busk, J., Schmidt, M. N., Winther, O., Vegge, T., and Jørgensen, P. B. Graph neural network interatomic potential ensembles with calibrated aleatoric and epistemic uncertainty on energy and forces. *Phys. Chem. Chem. Phys.* **25**, 25828 (2023)

[138] Raccuglia, P. *et al.,* Machine-learning-assisted materials discovery using failed experiments. *Nature.* **533** (7601), 73–76, 10.1038/nature17439 (2016).

[139] Tardif, S. *et al.,* Combining operando X-ray experiments and modelling to understand the heterogeneous lithiation of graphite electrodes. *Journal of Materials Chemistry A.* **9** (7), 4281–4290, 10.1039/D0TA10735B (2021).

[140] https://MaterialsCommons4.eu – Driving Digital Innovation in Materials Science within Europe.

[141] Maaløe, L., Fraccaro, M., Winther, O. *Semi-Supervised Generation with Cluster-aware Generative Models.* arXiv Prepr. arXiv1704.00637 (2017).

A key advance needed to establish BIG is the design of standardised testing protocols for battery materials and cells to allow extraction of critical information regarding battery interfaces (and bulk properties) by comparing cell performance with cell chemistry. Guidelines should be defined for that purpose, becoming the project's characterisation quality label. This checklist should be aligned and complement previously published ones by scientific journals or other recently published large-scale initiatives to ensure interoperability within the scientific community. BIG represents a unique opportunity to design a common European strategy in which experimental data on each new chemistry, successful or not, will feed into a common data infrastructure that will be broadly accessible, for example, by a central AI orchestrating the materials discovery. To meet the challenges of standardising experimental data and observables as input to physical models, implementing feedback processes may be considered pivotal. This will be achieved by creating a European database of battery-oriented material properties and a standardised classification of interfacial phenomena, as well as by defining common observables for physical modelling used to initiate paths and feedback loops for the multi-scale integration of datasets and modelling. In this respect, a key role will be played by making workflows interoperable. Many workflow engines, such as *AiiDA*, *Pyron*, PerQueue[142], and *Jobflow*, as well as experimental platforms like *FINALES* and Aurora, have been implemented and used to orchestrate simulations and experiments. These methods cannot remain standalone efforts and require a common workflow standard, which would also integrate with other initiatives, such as the MaterialsCommons4EU discussed above[143].

To support the standardization of testing protocols, platforms will be developed and opened to European partners to certify battery performance, helping to better integrate academia and industry. Therefore, standardization efforts should not be limited to electrochemical testing or materials properties but must also cover the manufacturing of battery components and battery assembly. A stepping stone toward this goal is the definition of an ontology for active materials synthesis and manufacturing steps[144].

To enable feedback processes incorporating physical insights from multiscale modelling, physical models, and multimodal characterization, implementation of standards regarding operando measurements, modelling, and simulation is also necessary. Finally, protocols for data sharing, storage, and analysis must be implemented efficiently to ensure the seamless transfer not only of metadata for electrochemical testing and characterization but also of analysed data generated using automated analysis tools[145].

AI-enhanced multi-scale/multi-feature approaches

Combining different computational and experimental tools will certainly be necessary to grasp the dynamics of the interface at different scales rather than a single physical property[146].

Through AI-based techniques linking BIG and MAP, complex cross-scale features and connections that are imperceptible to humans can be identified, expanding the domains where reliable predictions are possible. However, modelling interphases and probing their behaviour remains highly complex due to the diversity of underlying phenomena.

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[142] Simon K. Steensen, et al., The Necessity of Dynamic Workflow Managers for Advancing Self-Driving Labs and Optimizers, Advanced Intelligent Discovery, 202500067, (2025).
[143] https://materialscommons4.eu
[144] https://zenodo.org/records/15069341
[145] Svaluto-Ferro, E.et *al.,* Toward an Autonomous Robotic Battery Materials Research Platform Powered by Automated Workflow and Ontologized Findable, Accessible, Interoperable, and Reusable Data Management. *Batteries & Supercaps,* 10.1002/batt.202500155 (2025)
[146] Franco, A.A. *et al.,* Boosting Rechargeable Batteries R&D by Multiscale Modeling: Myth or Reality? *Chemical Reviews.* **119** (7), 4569–4627, 10.1021/acs.chemrev.8b00239 (2019).

We envision developing more accurate models that capture realistic interfaces, aging, and degradation processes, as well as complex design scenarios. This requires robust mathematical frameworks capable of coupling electronic, atomistic, and mesoscopic models with continuum-scale representations.

To master the intricate coupling of relevant length and time scales critical to battery systems, integrated experimental and computational workflows will combine advanced multi-scale modelling, machine learning, and data analytics. In parallel, more coordinated and integrated experimental approaches will be established to accelerate correlative characterizations and real-time multiparameter material mapping under well-defined and controlled conditions.

Furthermore, the development of inverse modelling techniques that translate experimental data back into model parameters will be pursued, enabling deeper understanding and predictive capability across scales.

2.5 Forward vision

Traditional trial-and-error–based materials optimisation starts from a known interface composition and structure, relying on human intuition to guide improvements in performance. The forward-looking vision, however, is to enable inverse materials/interface design, where desired performance goals define the composition and structure that best fulfil these targets, without a priori defining the starting composition or structure of the interface.

To develop and implement suitable models for the inverse design of battery interfaces, it is necessary to incorporate the relevant physical understanding and the model capable of performing an inverse mapping from the desired properties to the original composition of the materials and external parameters/conditions. The generative deep-learning models described in Chapter 1 represent an efficient way to optimise the data flow and build the required bridges between different domains, helping solve the biggest challenges of battery interfaces (Figure 4).

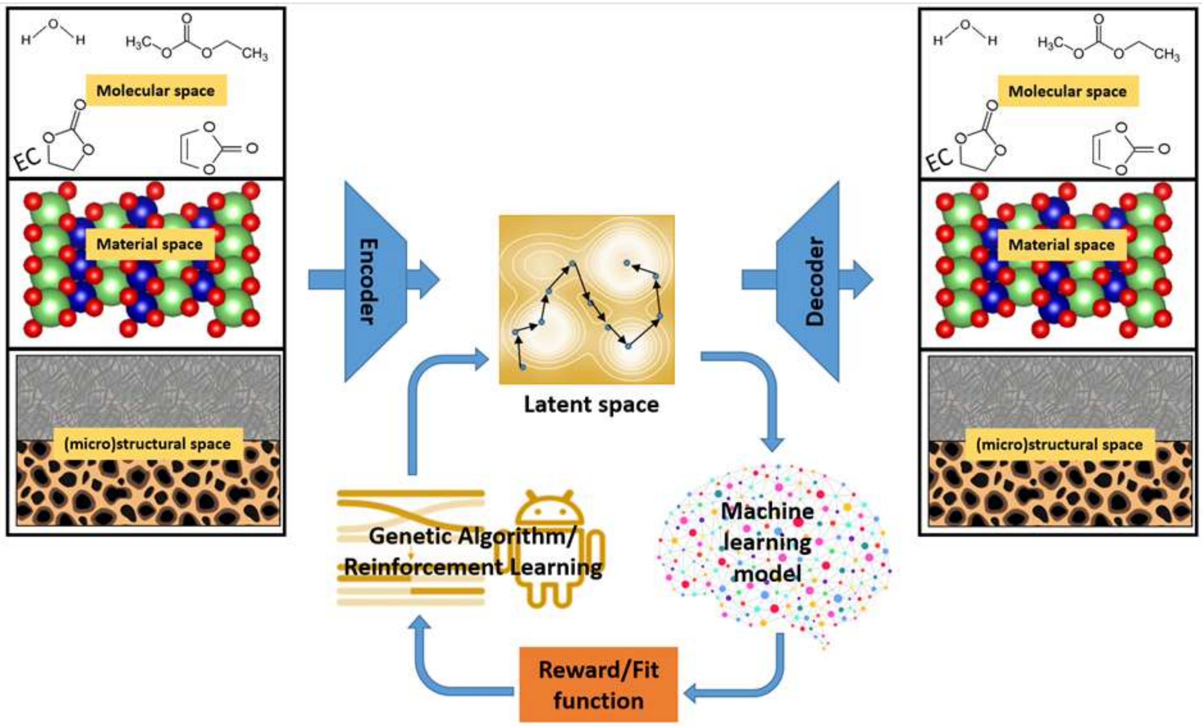

FIGURE 4. Generative model of interphase design. Variational auto encoder (VAE)-based encoding and decoding of chemical and structural information on a battery interphase into latent space, to enable

generative battery interphase design using, e.g., genetic algorithms or reinforcement-learning–based exploration[147]. Reprinted from Energy Storage Materials[148].

Inverse design strategy

This reliance on statistical correlations renders descriptors an ideal tool for data-driven AI methods. A promising approach is the full integration of data-driven methods and physical- based simulations. For example, inverse modelling with experimental datasets can reliably determine the interface descriptors that govern the detailed spatio–temporal evolution.

Based on these, forward simulations give insight into the expected spatially resolved time evolution of the system. With the outlined approaches, this finite number of parameters/features can be extracted by combining many simpler experiments using modern mathematical inverse modelling techniques and extracting a continuous four-dimensional spatio–temporal field of physical variables that can then be reduced to determining a finite set of parameters.

By doing this, rather than the empirical development of battery chemistry and assembly, which has been the norm so far, we aim to develop inverse battery design driven by data input which will also benefit the investigation of both production and recycling processes. This will be done sequentially to achieve, within ten years, a fully autonomous and automated platform, integrating computational modelling, material synthesis and characterisation, battery cell assembly, and device-level testing. Finally, we envision the battery discovery platform and the battery itself as fully autonomous, utilising, for example, the sensors developed in Chapter 3.1. to send signals that can be understood by the central BIG–MAP AI to predict the spatio–temporal evolution of the interface. If the model predicts a potential failure at the interface, this will launch the release of self-healing additives, as developed in Chapter 3.2, to pre-emptively heal the interface and possibly increase the battery lifetime. Furthermore, the development of such an inverse design strategy will also benefit the investigation of both manufacturing (Chapter 5) and recycling processes (Chapter 6).

Since the BIG–MAP project was not prolonged, the full implementation/timeline described the previous Roadmap 1.3 had to be revised. Below the revised goals for BIG.

In the short term (2025-2027): To integrate interphase data from *operando* synchrotron and other techniques developed in the BIG with experimental and simulation data from the MAP, including automated synthesis and cell assembly. This will utilize European data infrastructures like the European Battery Data Space and the BIG-MAP and CAPeX archive at DTU (achive-capex.energy.dtu.dk), and the Materials Cloud Archive (https://www.materials cloud.org) at EPFL to enable secure, interoperable data sharing and collaboration. Battery 2030+ initiative prioritises validating new methods on LIBs before extending to sodium-ion, solid-state, and other post-lithium chemistries. This effort is supported by the common central data infrastructure established by the European Commission, facilitating data-driven discovery and reproducibility across Europe.

The project will also investigate electronic configurations after ultrafast photoexcitation using Mn K-edge time-resolved X-ray absorption (trXAS), emission (trXES), and resonant emission spectroscopy (trRXES). Experiments will be conducted at XFEL and SACLA, supported by computational resources such as the DTU supercomputer, MareNostrum, and LUMI.

In the medium term (2027–2030): To extend characterization and modelling efforts to full-cell architectures and complex material stacks. Interlayer materials and processing strategies will be optimized using feedback from advanced modelling. Multiscale simulation frameworks will be expanded to include additional physical phenomena such as mechanical stress, swelling, and porosity evolution. Simultaneously, standardized experimental and modelling protocols for interface evaluation

[147] Nørskov, J.K., Bligaard, T., The catalyst genome. *Angewandte Chemie International Edition.* **52** (3), 776–777, 10.1002/anie.201208487 (2013).

[148] Bhowmik, A. *et al.,* A perspective on inverse design of battery interphases using multi-scale modelling, experiments and generative deep learning. *Energy Storage Materials.* **21**, 446–456, 10.1016/j.ensm.2019.06.011 (2019).

will be developed, with a strong focus on directly linking interface behaviour to key functional performance parameters, including cycle life and voltage stability.

In the long term (2030 and beyond) To develop predictive multiscale frameworks for designing and optimizing interfaces in battery systems. *Operando* data will be integrated into real-time simulations, enabled by comprehensive databases that combine structural, electrochemical, and metadata from *operando* studies. This integration will support real time simulations and digital twin development to support advanced cell design processes. Interface design will become a standard and critical step in battery development, alongside the choice of chemistry and architecture. Battery 2030+ aims to contribute actively to regulatory frameworks and industrial standards for interface stability and diagnostics. Ultimately, these advances will enable rational interface engineering across a wide range of systems, including solid-state, multivalent, and next-generation battery chemistries.

Understanding and controlling interfaces and interphases is essential for next-generation battery systems. The Battery 2030+ initiative has taken major steps in this direction through the coordinated efforts of OPERA, OPINCHARGE, and ULTRABAT. Yet, much work remains to bridge the gap between observation and design. In the next phase, the Roadmap must prioritise multiscale modelling, full-cell relevance, and integration of modelling with *operando* tools. Only then can we move from passive observation of degradation to active design of durable and efficient interfaces — tailored for the battery technologies of the future.

3. BATTERY SENSING, MANAGEMENT AND SELF-HEALING

As battery technologies evolve to meet the demands of performance, safety, and sustainability, the concept of the “smart battery” is emerging as the key pathway of technological progress beyond traditional routes of material or engineering approaches. This concept refers to a battery system equipped with sensors, self-healing functionalities and BMS to monitor and optimize performance, ensure safety, extend lifespan, and enable predictive maintenance. Sensing and self-healing are closely linked and central to the vision of smart batteries. Data acquired by sensors will be analysed by the Battery Management System (BMS), which can trigger a self-healing response when the maximum or threshold value of a detected (sensed) characteristic is reached. Battery 2030+ has played a central role in establishing a coordinating research effort under its umbrella in the past three years. However, the implementation of self-healing functionalities requires a multidisciplinary approach where self-healing, sensing, BMS and manufacturing are co-developed, and Europe still needs solid steps in this regard. The overall success of a smart battery will depend on designed synergy between sensing, BMS, and self-healing (Figure 5).

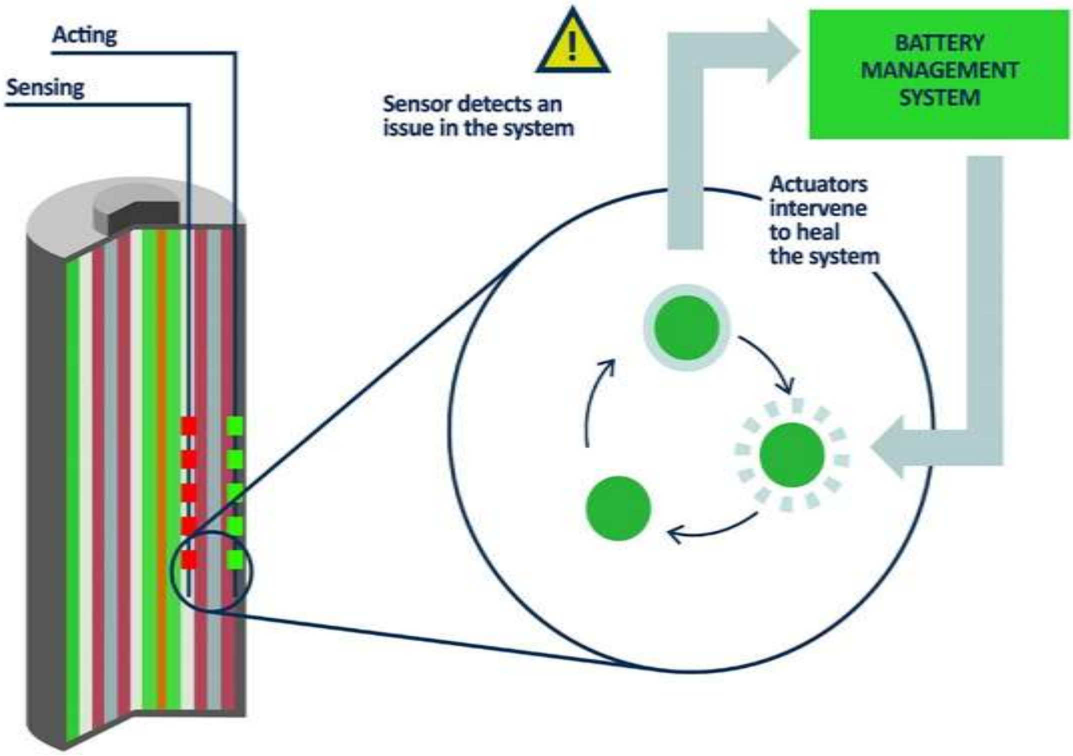

FIGURE 5. The synergy between sensing, BMS, and self-healing.

Smart functionalities such as embedded sensing, adaptive control, and self-healing mechanisms have the potential to significantly enhance existing battery operation, monitoring and lifetime management. Within Battery 2030+, the vision in this area, is to move from passive energy storage devices toward self-aware systems that can sense internal states, respond to degradation, and autonomously adapt their performance through advanced battery management. This includes the development of new functionalities for the BMS, such as integrating sensors, advanced data management, new state-of-X models, self-healing mechanisms, and linking the physical BMS with a virtual BMS through digital twin technologies.

The projects **PHOENIX**, **SALAMANDER**, **HEALINGBAT**, **INERRANT**, and **SAGELi** are the current drivers of this transformation. Their work spans the development of embedded and wireless sensors (e.g., for temperature, pressure, gas evolution, metal ion release, impedance), self-healing components (e.g., binders, separators, electrolytes), and diagnostic interfaces for modular BMS systems. Some demonstrators are already being tested in 1Ah baseline cells, offering a promising foundation for future scale-up.

Despite this progress, the full potential of smart functionalities remains to be unlocked. Many sensing solutions are still in the proof-of-concept stage. The self-healing mechanisms often lack validation in practical cells or long-term cycling conditions. The combination of these elements — sensors, healing, and intelligent BMS control — into a coherent, closed-loop system remains largely conceptual. The path toward widespread deployment requires clear definitions, robust integration strategies, and validation at scale.

For sensors, a myriad of technologies exists: the quantifiable connection between the signal they obtain and the degradation mechanism they are meant to track is one of the many challenges for sensor technology as applied to batteries. On the one hand, the maturity of sensor technology means many new parameters about batteries can be measured by implementing sensors; on the other hand, understanding of how to best interpret their data is lacking. The questions of sensor integration in the cell manufacturing is a major challenge for smart batteries in addition to calibration, sensitivity, and, if necessarily inside the cell, encapsulation or chemical compatibility.

For self-healing, the technology must evolve from a passive material property to an active, system-level function. Its durability and chemical compatibility must be at the same standard as other battery material components. The functionality of self-healing introduces many new parameters, interfaces, and interactions which could interfere with battery operation as much as they enhance it. Therefore, integration of a self-healing functionality into a battery cell is a clear challenge, but one with substantial benefits to performance if successful.

3.1 Introduction

The BMS is the bridge and the “brains” of a smart battery that enables both sensors and self-healing to work together (Figure 5). Seamless integration of sensor data with the BMS is necessary for their usability. Sensor outputs must inform not only diagnostics but also real-time operational decisions. This calls for the development of next-generation BMS architectures that are modular, adaptive, and scalable, capable of processing diverse inputs and responding dynamically to degradation signals. Ultimately, the vision is to trigger healing responses based on specific degradation signatures detected via sensing, coordinated and governed by the BMS. This feedback-driven approach could significantly extend battery lifetime and reduce the need for conservative design margins.

These three elements of sensor, self-healing, and BMS can be demonstrated at the lab- or prototype-scale. Smart functionalities and sustainability must be evaluated not only for their technical benefits but also for their impact on cell design, production complexity, cost, and recyclability. Integration of novel materials and embedded components must be compatible with scalable industrial processes: this aspect is non-negotiable if there is any expectation for smart functionalities to be implemented into real-world products. Technologies that show promise in laboratory-scale coin cells must prove effective in pouch or cylindrical formats, under realistic cycling, ageing, and environmental conditions. Only then can they transition toward market adoption.

Finally, predictive diagnostics and virtual sensing offer promising paths to reduce complexity. Through data fusion and machine learning, it may become feasible to infer internal battery states from indirect measurements, reducing the need for physical sensors in every unit and opening the door to more streamlined, cost-effective smart systems.

Together, these efforts will define the next generation of intelligent battery technologies—aligning with the Battery 2030+ vision of safe, sustainable, and high-performance energy storage solutions tailored for the future.

Smart functionalities are becoming a key enabler for next-generation batteries that last longer, fail less often, and communicate with their surroundings. Battery 2030+ is laying the groundwork for this transformation, but the journey has just begun. The next Roadmap phase must focus on integration: merging sensors, healing materials, and BMS systems into a coherent functional unit, validated under real-world conditions. In doing so, Europe can lead the global transition to batteries that are not just better — but smarter.

3.1.1 Integration of smart functionalities: Sensing

Our increasing dependence on batteries calls for the accurate monitoring of battery functional status so as to increase their quality, reliability, and life (QRL)[149,150]. In recent decades, numerous on-board electrochemical impedance spectroscopy (EIS) devices and sophisticated BMSs have been developed for this purpose, but with limited success. Whatever battery technology is considered, its performance is governed by the nature and dynamics of the interfaces within the battery cell, which in turn rely on temperature-driven reactions with unpredictable kinetics. Although monitoring temperature is essential for enhancing battery cycle life and longevity, this is not directly measured today at the cell level in running Electric Vehicles (EVs) or in development setups, where the fine-tuning of the battery pack is developed.

Drastically enhancing battery cell QRL calls for better knowledge/monitoring of the physical parameters during cycling and an understanding of the science beyond the parasitic chemical processes taking place within the battery cells.

The long-term vision for the Battery 2030+ initiative is to transform the battery from a simple "black box" into an intelligent, transparent system. Achieving this requires a hierarchical approach at both the component and full system levels. Embedding smart functionalities within the battery cell can be realized through the integration and development of diverse sensing technologies capable of transmitting information into and out of the cells. Of particular importance are sensors that provide spatially resolved monitoring—measuring multiple parameters at various locations within a cell. Key parameters include temperature (T), pressure (P), strain (ε), electrolyte and SEI composition, lithium plating, electrode breathing (ΔV), electrode potential, gas evolution, and heat flow, all measured with high sensitivity.

For practical implementation, the adaptability of these sensing technologies must be carefully considered, accounting for the chemical environment within the battery as well as manufacturing constraints. To this end, the scalable, low-cost manufacturability of miniaturized sensing technologies is a prerequisite for their deployment at large scale. Equally important is ensuring effective processing and transmission of the sensing data. To challenge the existing limitations, we propose a disruptive approach of injecting smart embedded sensing technologies and functionalities into the battery cell,

[149] Narayan, R., Laberty-Robert, C., Pelta, J., Tarascon, J.-M., Dominko, R., Self-Healing: An Emerging Technology for Next-Generation Smart Batteries. *Advanced Energy Materials*, 2102652, 10.1002/aenm.202102652 (2021).
[150] Berecibar, M., Machine-learning techniques used to accurately predict battery life. *Nature.* **568** (7752), 325–326, 10.1038/d41586-019-01138-1 (2019).

capable of performing spatial and time-resolved monitoring (see Figure 6)[151].

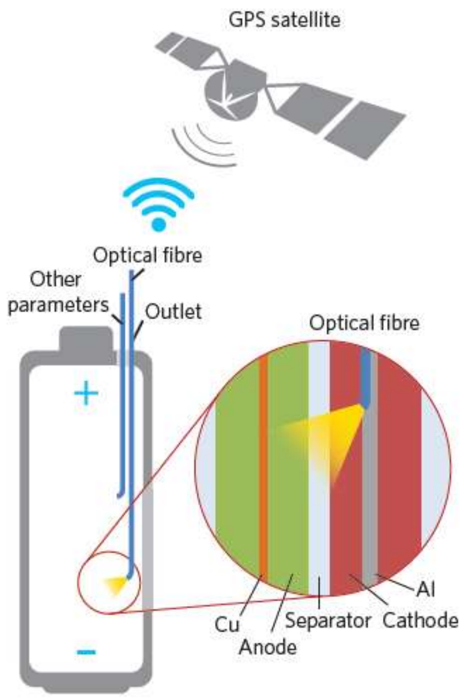

Figure **6**. A future battery with an output analyser connected to sensor (optical fibres, wires, etc.) in addition to the classical positive and negative electrodes.

A critical challenge is to identify reliable state function estimators and develop robust algorithms that can intelligently interpret the vast amount of sensing data. This will enable the creation of responsive, smart battery management systems. Close collaboration with the FULL-MAP component of this Roadmap is essential to successfully realize this vision.

3.1.2 Current Status

Over the years, many fundamental studies have examined different battery chemistries using sophisticated diagnostic tools such as X-ray diffraction, nuclear magnetic resonance (NMR), electron paramagnetic resonance (EPR), and transmission electron microscopy (TEM), which can ideally operate *in situ* and even *operando* as the battery is cycled[152]. Although these analytical techniques are quite advanced, they rely on specialized equipment and cells that cannot be easily transferred to analysing commercial cells. In contrast, lithium distribution density and structural effects were recently imaged in 18650 cells; however, the imaging techniques used depend mainly on large-scale facilities with limited access [153] . Notable progress has been made over the years towards instrumental miniaturisation, so that bench-top X-ray diffraction units, scanning electron microscopes, and portable impedance (and even NMR) spectrometers exist, but we are still far from producing the test units needed to monitor batteries in their end applications. These types of advances towards monitoring the battery's functional status in real time is still unmet.

Determining the state of charge (SoC) of batteries has been a challenging issue almost as long as batteries themselves have existed. Over the years, this challenge has led to a wide variety of monitoring approaches and patents covering various sensing technologies (Figure 7). For decades,

[151] Vegge, T., Tarascon, J.-M., Edström, K., Toward Better and Smarter Batteries by Combining AI with Multisensory and Self-Healing Approaches. *Advanced Energy Materials*. **11** (23), 2100362, 10.1002/aenm.202100362 (2021).
[152] Grey, C.P., Tarascon, J.M., Sustainability and in situ monitoring in battery development. *Nature Materials.* **16** (1), 45–56, 10.1038/nmat4777 (2016).
[153] Senyshyn, A., Mühlbauer, M.J., Nikolowski, K., Pirling, T., Ehrenberg, H., "In-operando" neutron scattering studies on Li-ion batteries. *Journal of Power Sources.* **203**, 126–129, 10.1016/j.jpowsour.2011.12.007 (2012).

research in this area focused primarily on lead-acid (Pb-acid) battery technology, aiming to make it more reliable and user-friendly. Significant progress was made with the implementation of Electrochemical Impedance Spectroscopy (EIS), an elegant tool used to evaluate changes in cell resistance during cycling in Lead-acid (Pb-acid) batteries, thereby enabling estimation of their state of health (SoH).[154] Portable EIS devices have since been commercialized and are used in transportation and telecommunications backup systems to identify faulty batteries within modules. However, these devices still suffer from limited reliability, typically below 70%. Overall, accurate State of Charge (SoC) monitoring remains highly challenging, and no fully reliable solution currently exists. Today's SoC estimation typically relies on a combination of direct measurements such as EIS, resistance measurements, current pulse tests, coulomb counting, and open circuit voltage-based methods.

As batteries become increasingly central to daily life, the demand for highly reliable and long-lasting batteries has intensified. This has reinvigorated battery sensing research, leading to novel approaches for passively monitoring parameters such as temperature, pressure, strain, and the dynamic change (ΔV) of the SEI. These methods often rely on non-destructive sensors including thermocouples, thermistors, pressure gauges, and acoustic probes.

However, most current sensing activities rely on sensors positioned outside the battery cells, which limits knowledge to macroscopic properties while overlooking internal chemical and physical parameters crucial for monitoring battery lifetime. Consequently, implantable sensors are attracting increasing interest, with optical sensing technologies being predominant. Recent studies have highlighted the advantages of fibre Bragg grating (FBG) sensors and other implantable sensors for: i) accurately monitoring temperature, pressure, and strain during cycling, ii) imaging cell temperature distribution, and iii) estimating battery SoC without interfering with cell performance.

The time has come to move beyond conceptual demonstrations and address the remaining challenges to make non-invasive, internal battery sensing a practical reality. Industry requires comparable and traceable reference methods to accurately assess battery state. This goal should be pursued by developing standardized measurement methods and procedures that advance SoC and SoH evaluation according to best metrological protocols, as outlined by organizations such as the European Association of National Metrology Institutes (EURAMET)[155].

3.1.3 Challenges

Numerous sensing technologies for battery modules and systems have been tried (see Figure 7) and it is outside the scope of this Roadmap to list them all; rather, our intent is to highlight the ones with the greatest chances of success at the battery cell level.

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[154] Keddam, M., Stoynov, Z., Takenouti, H., Impedance measurement on Pb/H2SO4 batteries. *Journal of Applied Electrochemistry.* **7** (6), 539–544, 10.1007/bf00616766 (1977).

[155] EURAMET - European Association of National Metrology Institutes, Documents & Publications - EURAMET, https://www.euramet.org/publications-media-centre/documents/?L=0, accessed 22 August 2023.

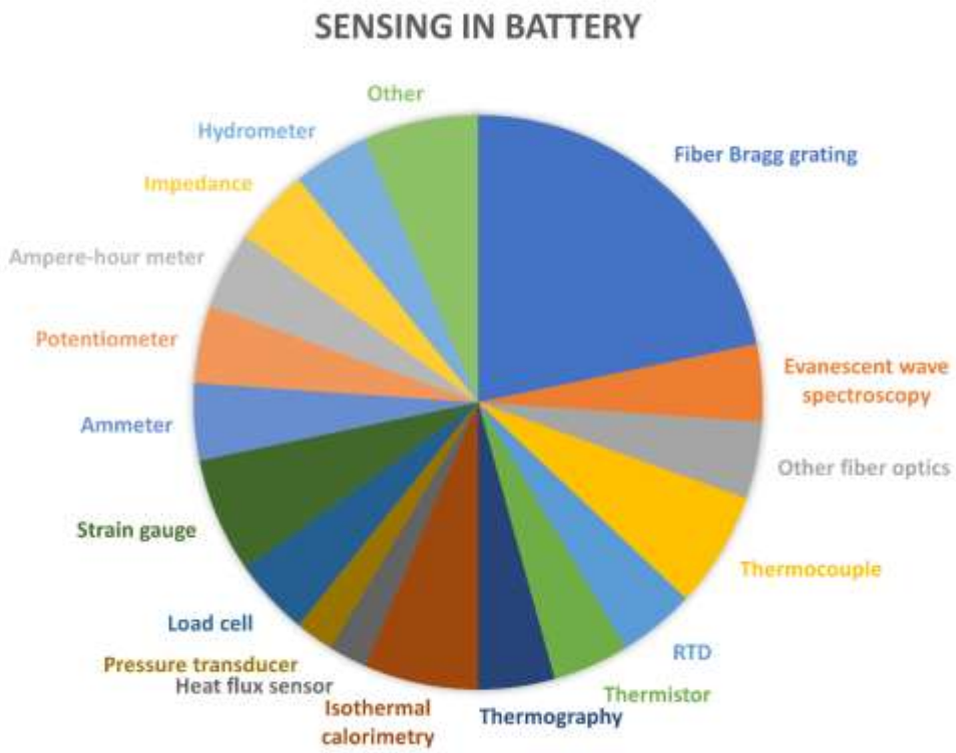

FIGURE 7. A summary of available sensing technologies for battery modules and systems, with data reflecting the number of relevant published articles for each technique found in the 2019 bibliography.

Temperature Sensors

Surface temperature measurement at a single location on a battery cell has long been used to validate thermal battery management system (TBMS) models. Temperature sensors generally fall into four main categories: resistance temperature detectors (RTDs), thermally sensitive resistors (thermistors), thermocouples, and FBG optical sensors. These sensors differ in accuracy and in how conveniently they can be positioned within the cell. For example, thermistors, due to their thickness (~1 mm), are typically positioned only on the top surface of the cell rather than directly on it, unlike thinner RTDs (~100 µm)[156].

Interestingly, longitudinal surface temperature variations during operation have been mapped with an accuracy of ±1°C by screen-printing thermal sensor arrays on the surface casing of 18650 cylindrical cells. However, the scarcity of information regarding the inside of the cell limits the integrity of current TBMS models, calling into question their accuracy and predictive capabilities. Simplified attempts to alleviate this issue have involved implanting thermocouples within 18650 and pouch cells. A notable achievement is the successful "electrocardiogram" of a 25Ah battery, realised by embedding 12 thermocouples at specific locations within cells, along with 12 additional ones at the corresponding positions on the cell surface. This configuration allowed temperature contours within the cell to be plotted, providing valuable information to validate thermo–electrochemical models. However, drawbacks of this approach include the challenges of positioning multiple thermocouples and wiring them without compromising the tightness of the cell and its performance. A more convenient way to assess temperature contours and identify hot spots within the cell is infrared thermography, but this technique suffers from poor spatial resolution, limited temperature accuracy, and susceptibility to background noise.

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[156] Knobloch, A. *et al.,* Fabrication of Multimeasurand Sensor for Monitoring of a Li-Ion Battery. *Journal of Electronic Packaging.* **140** (3), 10.1115/1.4039861 (2018).

Gauge sensors (ε, P)

Monitoring temperature, sensing intercalation strain and cell pressure are equally critical for tracking SEI dynamics and phenomena such as lithium plating, which directly affect the SoC and SoH of batteries. Early experiments utilized *in situ* strain gauge measurements to probe total volume changes during the charging and discharging of Nickel–Cadmium (Ni-Cd) batteries. This approach was later extended to commercial Li-ion and lithium cobalt oxide/graphite (carbon) battery cell systems ($LiCoO_2$/C) alongside other chemistries to measure strain associated with phase transitions, as well as to quantify delays in cell volume variation as a function of cycling rate. Using a strain sensor placed on the cell surface, Dahn et al. demonstrated that irreversible volume expansion caused by SEI growth could be detected by *operando* pressure measurements. They further established a correlation between capacity retention and irreversible pressure increase[157]. The simplicity of this method, relying solely on external sensors, is a key advantage. However, the use of single sensors can create mechanical pressure points during bracing, which negatively impacts battery lifespan. Therefore, a soft, fully surface-mounted sensor solution with spatial resolution is required to overcome these limitations.

Electrochemical sensors

Typically, the electrochemical (voltametric, amperometric) cell/system used in the laboratory can be viewed as electrochemical sensors for detecting various species, but an inherent drawback for use in battery sensing is miniaturisation issues. This is changing owing to recent advances in the field of biophysics/chemistry, so that electrochemical sensors are now suitable for miniaturisation down to micro or even nano-dimensions using several mechanical, chemical, and electrochemical protocols to prevent environmental artifacts (e.g., convection). The combination of advanced electrochemical (pulse) techniques and unique suitability for electrode/sensor miniaturisation and electrode modification provides an excellent basis for designing powerful new detection microsystems that could be conveniently incorporated into batteries provided that remaining material aspects can be resolved. Partially that has been demonstrated by printing technology where electrodes and sensing layer can be printed on different substrate and sensing is achieved by measurement of difference in the physico-chemical properties of sensing layer (for instance change in resistance or capacitance of the sensing material that can be monitored by impedance measurements).

A persistent challenge in electrochemical battery diagnostics is the development of effective, (electro)chemically stable, and durable (quasi-)reference electrodes (REs) suitable for voltametric, amperometric, and/or potentiometric detection regimes. REs are of paramount importance for understanding battery chemistries at the laboratory scale, where only a few tens of cycles are typically needed to identify failure mechanisms and other limitations. They enable: (i) identification of the distinct contributions of each cell component to the overall battery performance; (ii) correct interpretation of current and voltage data with respect to individual components; and (iii) investigation of the reaction mechanisms at each electrode. However, challenges remain in: (i) selecting an RE composition that ensures chemical inertness within the cell environment; and (ii) defining an optimal RE geometry and placement relative to other cell components—both of which depend on the specific cell configuration and are critical to avoiding experimental artifacts. The integration of REs into battery sensing is therefore an attractive approach. Yet, it must be acknowledged that, to date, no reliable, user-friendly, chemically stable, long-lasting, and artifact-free cell configurations are available. Developing such solutions remains an open and important task.

Optical sensors

FBG sensors, which correlate the wavelength dependence of the emitted signal with local temperature, pressure, and strain, are by far the most studied type of optical fibre sensor. Few

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[157] Louli, A.J., Ellis, L.D., Dahn, J.R., Operando Pressure Measurements Reveal Solid Electrolyte Interphase Growth to Rank Li-Ion Cell Performance. *Joule.* **3** (3), 745–761, 10.1016/j.joule.2018.12.009 (2019).

research groups have shown how FBG sensors could be used to volumetric expansion radial map a commercial cylindrical LiB and to thermally map a battery pack during operation[158]. Moreover, PARC (a Xerox company) has demonstrated the feasibility of obtaining high-performing Li-ion pouch cells for EV applications with embedded FBG sensors attached to the electrode while not observing major adverse effects of the embedded fibre on the cell life for at least 1000 cycles[159] Based on the accuracy of the strain measured using FBG sensors, the SoC was estimated with less than 2.5% error under different temperature conditions and under dynamic cycling. The authors could predict the cell capacity up to ten cycles ahead with approximately 2% error. However, a difficulty with FBG use is that it simply decouples[160,161]. Nevertheless, they require a more expensive interrogation system and greater calculation resources to analyse the large amount of data generated.

A solution to this decoupling issue has been provided by the arrival of micro structured optical fibres (MOFs)[162]. Unlike FBG sensors, whose functioning relies on a change in refractive index (RI) between core and cladding to obtain total internal reflection of light, MOFs achieve total internal reflection by the manipulation of their waveguide structure, enlisting air holes within the fibre core whose patterning determines the specific properties of MOF sensors. Hence, with careful design of the air-hole pattern, MOFs offer a feasible way to measure temperature and pressure independently with a single fibre. However, MOF fabrication is still in its early research stage.

Alternatively, hybrid sensing configurations based on Fabry-Perot interferometers and FBG sensors have been recently developed to internally track and discriminate in real time temperature and pressure variations on commercial Li-ion cylindrical batteries[163, 164].

Nano-plasmonic sensing (NPS)

NPS introduced to the field of batteries as recently as 2017, has the advantage of focusing, amplifying, and manipulating optical signals via electron oscillations known as surface plasmons (SPs). NPS technology relies on the shift in the wavelength of the plasmon resonance peak, due to a change in the RI of the surrounding medium nearest (<100 nm) the sensor surface. These sensors can then be used for the *in-operando* monitoring of physicochemical phenomena occurring on the nanoscale, such as SEI growth, lithium intercalation/deintercalation, and local ion concentration variations[165].

However, making such sensors requires the deposit of a metallic plasmonic nanostructure on top of the fibre, whose physicochemical stability upon cycling in presence of electrolytes remains undetermined.

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[158] Matuck L. *et al.,* Customized Optical Fiber Birefringent Sensors to Multipoint and Simultaneous Temperature and Radial Strain Tracking of Lithium-Ion Batteries. *Advanced Sensor Research.* **2** (7), 10.1002/adsr.202200046 (2023).

[159] Raghavan, A. *et al.,* Embedded fiber-optic sensing for accurate internal monitoring of cell state in advanced battery management systems part 1: Cell embedding method and … *Journal of Power Sources* (341), 466–473, 10.1016/j.jpowsour.2016.11.104 (2017).

[160] Huang, J. *et al.,* Operando decoding of chemical and thermal events in commercial Na(Li)-ion cells via optical sensors. *Nature Energy.* **5** (9), 674–683, 10.1038/s41560-020-0665-y (2020).

[161] Huang, J., Blanquer, L.A., Gervillié, C., Tarascon, J.-M., Distributed Fiber Optic Sensing to Assess In-Live Temperature Imaging Inside Batteries: Rayleigh and FBGs. *Journal of The Electrochemical Society.* **168** (6), 60520, 10.1149/1945-7111/ac03f0 (2021).

[162] Mei, W., *et al*., Operando monitoring of thermal runaway in commercial lithium-ion cells via advanced lab-on-fiber technologies. *Nature Communications* 14, 5251 10.1038/s41467-023-40995-3 (2023).

[163] Matuck L. *et al*., Towards smart and secure batteries: Linking pressure and temperature profiles with electrochemical behavior through hybrid optical fiber sensors, *Chemical Engineering Journal*, 500, 10.1016/j.cej.2024.156806 (2024).

[164] Matuck, L. Ferreira, M.S., and Nascimento, M. Revealing a Correlation between Physical Parameters and Differential Voltage Analysis of a Commercial Li-Ion Battery Based on Fiber Optic Sensors, *Batteries*, **10**, 289, 10.3390/batteries10080289

[165] Lao, J. *et al.,* In situ plasmonic optical fiber detection of the state of charge of supercapacitors for renewable energy storage. *Light: Science & Applications.* **7** (1), 34, 10.1038/s41377-018-0040-y (2018).

Acoustic sensing

Batteries are breathing objects that expand and contract upon cycling, with volume changes as great as 10%. This leads to significant mechanical stress (i.e., cracking) inside the battery's materials, which can generate acoustic signals. "Listening" to and analysing the elastic acoustic waves generated by battery materials during operation has long been considered potentially useful for battery studies.
The acoustic emission (AE) technique is used to monitor numerous types of battery chemistries (e.g., Pb-acid and Nickel–Metal Hydride battery (Ni-MH)) and was more recently implemented in the study of LIBs during the formation stage. However, AE has some important limitations, including the minimum threshold stress required to generate acoustic waves and the lack of spatial recognition as a sensing technique.
In contrast, AE is very effective for: studying the formation step of batteries; detecting operating conditions that lead to excessive stress on the battery's materials; detecting early signs of abnormal behaviour that could lead to safety issues.
Acoustic sensing via ultrasound transmission is another promising method for advanced State of X (SoX)[166] monitoring. By measuring the time of flight of ultrasonic acoustic waves—generated by piezoelectric transducers and propagating through the battery—a direct relationship to SoC and SoH can be observed. In addition, the attenuation of the signal is highly sensitive to SoC as well.

Gas sensors

The monitoring of gas evolution is of interest both in-situ, e.g. to detect changes on the chemical composition of the electrolyte as well as ex-situ to herald leakages from battery cells. Gas sensing approaches in general are characterized by a plethora of different technologies, which requires an application-specific assessment in terms of selectivity, stability, and sensitivity. In particular, the wealth of possibly relevant gas species scales with the various battery chemistries and currently, no single low-cost gas sensing technology has emerged that is able to cover all applications. In basic research, analytical equipment is typically employed for in-depth characterization of the gas composition. Approaches for monitoring gas composition pursued to date mostly rely on analysing extracted gas samples, which is inherently unsuitable for real-time monitoring. In-situ methods have hardly been used so far, in part because technologies that may be miniaturized are neither stable nor selective enough for most real-world applications. Instead, technologies have been used which cannot be miniaturized and are therefore conceptually unsuitable for real-time, in-situ investigations. Current research is mostly performed using Fourier transform infrared spectrometers (FTIR)[167] including DRIFT[168], X-ray photoelectron spectroscopy (XPS)[169], and electrochemical mass spectrometry (DEMS)[170]. None of the approaches used in research to date are suitable for microintegration.

Standardization

The integration of sensing functionalities into battery cells and packs requires seamless communication between sensors and the BMS[171]. Establishing standards for data generation, transmission, and interpretation—combined with a smart BMS—will enable improved lifetime, safety, and faster charging through enhanced process understanding and reproducibility. Standardized protocols must cover both data and metadata reporting.

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[166] SoX is an umbrella term for different "state indicators" (charge, health, power, energy) that describe a battery's status.
[167] M. Dollé, *et al. J. Power Sources* **97-98,** 104–106 (2001)
[168] M. A. Teshager, *et al. ChemElectroChem* **3,** 337–345 (2016)
[169] S. Wenzel, S., Solid *State Ion.* **278,** 98–105 (2015)
[170] Biasi, L. de *et al. ChemSusChem* **12,** 2240–2250 (2019)
[171] Zeng, X., Berecibar, M. Emerging sensor technologies and physics-guided methods for monitoring automotive lithium-based batteries. *Communications Engineering.* **4**, 44 10.1038/s44172-025-00383-9 (2025).

Once comparability of sensor results is ensured, full connectivity with the BMS can be achieved. This involves integrating sensor connectivity and data management at the cell, module, and pack levels, while maintaining compatibility with battery manufacturing processes. A standardized process for sensor integration and BMS connection is therefore essential.

In summary, battery sensing is moving beyond proof-of-concept and is becoming critical to the design and monitoring of next-generation smart batteries. Achieving this vision requires mastering efficient sensor data processing and establishing robust communication between sensors and BMS systems. Communication interfaces must be treated as an integral part of the sensor and considered early in the co-design of both sensor and cell. Ultimately, sensor information should trigger autonomous BMS responses, based on validated cell and battery models, and enhanced by AI and machine learning. Realizing the full potential of this field demands advances in both hardware and software—topics addressed in the methods developed within the BIG-MAP and FULL-MAP initiatives of Battery 2030+.

3.1.4 Advances needed to meet the challenges

Our proposed disruptive approach to meeting these challenges is to introduce smart embedded sensing technologies and functionalities into the battery capable of performing the spatially and temporally resolved monitoring of changes detrimental to battery life. This long-term vision needs to be addressed hierarchically on both the component and full system levels.

Introducing smart functionalities into the battery will include the integration and development of various sensing technologies previously used in other research sectors, technologies that rely on optical, electric, thermal, acoustic, or even electrochemical concepts to transmit information into/out of the cells**.** Sensors that can measure with great accuracy multiple parameters such as strain, temperature, pressure, electrolyte concentration, and gas composition and can ultimately access SEI dynamics must be designed/developed. For the successful implementation of the sensing tooling in a practical battery, sensors will have to be adapted to the targeted battery environment in terms of (electro-)chemical stability, size, and manufacturing constraints, including recyclability.

The manufacturing constraints also include the consideration of system design trade-offs. The identified sensors have different requirements in terms of signal generation as well as data acquisition and processing. Optical and acoustic sensors require signal generation and dedicated data acquisition electronics, which are ideally positioned directly on the battery cell to avoid wiring. Moreover, these types of sensors required data acquisition in the several kHz or even MHz range, which puts severe constraints on the data communication with the BMS when considering multiple data streams required to support a high spatial resolution. The system design trade-offs include the analysis of local versus central data pre-processing and hardware requirements for associated data transmission volumes together with the overall techno-economic optimization of all required electronic components.

Addressing manufacturing constraints is no doubt important, but an urgently missing gap to achieve this is the lack of expertise on the practical implementation of sensors into cells and electrode-electrolyte components. While this expertise partially exists, it lies outside the battery community, and its transfer to battery environments is technologically challenging. For instance, optical sensors reliant on FBGs, and long-period fibre gratings (LPFGs) are commonly used in civil engineering for monitoring the health of structures such as bridges, buildings, etc. However, the adaptation of these technologies to the constraints of battery environments requires considerable development efforts. In another example, the insertion of FBGs into composites is an inherent part of assembling H_2 storage cylinders with the sensors being wired to monitor cracks. Because the transducing mechanisms are well-known, it would be more effective to launch open calls that engage the broader sensing community from both academic and industry. This strategy is crucial for Battery 2030+ in advancing battery sensing technologies. Notably, the real potential of optical sensing multiplexing has already been demonstrated, enabling the monitoring of multiple metrics through a single optical fibre, thereby reducing the wiring complexity.

For sensor development, there are two successive steps: the identification of suitable transducing mechanisms followed by the development and integration of new specific sensors dedicated to the battery. In both cases, it is important to ensure the metrological traceability of these sensors with regards to primary references in order to ensure comparable measurements and hence more meaningful experiments (see documentation by EURAMET, the European Association of National Metrology Institutes)[172].

For sensors incorporated directly into battery cells, the harsh chemical environment demands innovative chemical coatings with high chemical and thermal stability. Miniaturisation to the micron scale is essential so that sensors can fit within separator thicknesses without impairing cell performance. Optimizing the location and placement of sensors to balance accuracy and effect on electrochemical performance is also a needed advancement.

In alignment with Battery 2030+ manufacturing and recyclability objectives, a key manufacturing goal is to make sensors an intrinsic part of the battery, rather than an add-on. As with thermistors, printing-based fabrication processes could enable integration both inside and outside the cell, as well as on specific battery components, to allow true *in situ* measurements. Printing-based fabrication can also be readily scaled to roll-to-roll processes. Nevertheless, the material choice for sensors and their encapsulation should involve relevant experts to check for compatibility and other far downstream impacts on recycling processes, especially for more advanced recycling methods like direct recycling.

A major challenge in smart battery development is ensuring reliable data transmission in the battery's noisy electromagnetic environment, where excess wiring would drastically increase manufacturing costs and potentially offset sensor benefits. Possible solutions include wireless communication, power line communication using existing current-carrying wires, or multi-parameter sensors that combine optical sensing configurations without comprising performance.

To enable the commercial success of advanced sensor concepts, it is essential to demonstrate their economic benefits. Adding new sensors and the associated electronics involves upfront investments, which can be significant barriers for many price-sensitive battery applications. However, leveraging these sensors can deliver substantial performance improvements, such as significantly extended battery lifetime and more accurate estimates of SoC, SoH, System of Systems (SoS), and other SoX. These benefits translate into economic advantages over the battery's entire lifecycle. Therefore, it is crucial to identify, define, and quantify suitable economic performance indicators to support a cost-benefit analysis that motivates industry and end-user adoption of the technology.

Ensuring societal impact requires a systematic approach that closely connects the battery pack, BMS, and the application. Sensing technologies generate vast amounts of data, creating opportunities for AI-driven insights, but thoughtful integration of this data into the BMS is necessary to fully harness its potential. This integration will greatly benefit from the AI pillar of Battery 2030+, encouraging transversal collaboration to develop sophisticated BMS and TBMS systems that capitalize on the synergy between AI and sensing. A particularly promising concept is that of **virtual sensors**, as demonstrated in INSTABAT project, which utilises reduced-order cell models to estimate critical cell parameters in real time using data from physical sensors. Virtual sensors can significantly improve BMS functionality and can be implemented either directly in the physical BMS or in a virtual BMS in the cloud. The latter, enhanced through digital twin technologies, provides a powerful link to the MAP and BIG activities within the Battery 2030+ Roadmap. However, achieving successful data integration and effective linkage with AI require robust standardization, including standards for data transmission between sensors and AI systems, adoption of common data formats, and the implementation of protocols for data sharing and battery cycling.

[172] EURAMET - European Association of National Metrology Institutes, Documents & Publications - EURAMET, https://www.euramet.org/publications-media-centre/documents/?L=0, accessed 22 August 2023.

3.1.5 Forward vision

Within a ten-year horizon, the development of new sensors with high sensitivity, high accuracy, and low cost offers the possibility of access to a fully operational smart battery. The integration of this new technology at the pack level, with an efficient BMS having an active connection to an optional self-healing function, is the objective of the Battery 2030+ roadmap. Needless to say, realising this long-term vision of smart batteries includes several research facets with their own fundamental challenges and technological bottlenecks.

While recent projects have demonstrated significant results in cell instrumentation, very few investigations have addressed how sensors themselves behave over the entire lifetime of the battery, or how their presence might influence degradation pathways and safety profiles. Addressing these questions should be considered an additional short-term goal to ensure that sensing solutions are not only effective upon integration but remain reliable and non-intrusive throughout the battery's operational life.

In the short term (2025–2027): With the insights gained from the past three years, several medium-term goals outlined in the previous Roadmaps have become more attainable and are now reclassified as short-term goals. These include the miniaturization and integration of identified (electro)chemically stable, multifunctional sensing technologies—together with the necessary data processing and electronics—both at the cell level and within complete battery modules. This integration must be achieved cost-effectively and in alignment with industrial manufacturing processes.

Validating sensing accuracy for parameters such as SoC, SoH, resistance, and temperature under both calendar and cyclic ageing is essential. Sensors must also be capable of detecting and monitoring critical conditions in real time to enable early warning and preventive measures.

Due to recent progress, many results on cell instrumentation have already been demonstrated. However, there is still a notable lack of long-term studies on sensor stability over the battery's lifetime and the impact of sensors on cell ageing and safety. Addressing these gaps is critical to ensure that sensor integration not only delivers accurate measurements initially, but also remains reliable and non-invasive over extended operating periods.

Further priorities include prototyping modular BMS that can interface with sensor outputs, as well as exploring both the physical and economic integration of smart components into manufacturing workflows. It is crucial to validate the correlation between sensing-based detection of cell degradation and the activation of self-healing. In addition, the role of sensors in improving safety throughout the lifetime of the cell and the battery is to be thoroughly investigated.

In the medium term (2027–2030): To ensure the successful implementation of advanced battery systems, it is vital to demonstrate both the technical feasibility and economic viability for selected use cases. This involves integrating sensor connectivity and data management with the BMS at cell, module, and pack levels while ensuring compatibility with existing battery manufacturing processes. Additionally, demonstrating closed-loop systems (sensor/BMS/self-healing) in scalable battery formats at the module or pack level is essential.

Standardization of the sensor integration process and its connection to the BMS is crucial for streamlined operations, as well as establishing standardized test protocols for healing response, sensor calibration, and fault detection. Furthermore, developing AI-assisted diagnostic tools and virtual sensors will enhance predictive maintenance capabilities while minimizing the reliance on physical sensors.

It is equally important to adapt the reliability of the sensor integration and to establish design guidelines for integrating smart functionalities without compromising cell integrity or recyclability. This includes assessing the stability of sensors over the full battery lifetime and understanding their potential impact on cell ageing and safety—an area where long-term studies remain scarce despite significant recent advances in cell instrumentation.

Moreover, priority should be given to developing sensors capable of reliably signalling the true SoH or SoC, including low-cost solutions that can provide an unambiguous signal at the onset of critical events such as thermal runaway.

Lastly, evaluating the total cost of ownership and added value of smart batteries in key applications such as stationary storage, aviation, and mobility is critical for assessing their overall impact and viability.

In the long term (2030 and beyond): To achieve a fully operational smart battery pack, it is essential to master all aspects, including the economic trade-offs of data processing and transmission between sensors and an advanced BMS. Leveraging new data-driven AI approaches will facilitate the integration of sensing and monitoring advances with stimulus-activated local repair mechanisms, such as self-healing, in future cell designs and chemistries.

This integrated sensing–BMS–self-healing system will enable the development of smart batteries that continuously monitor, diagnose, and correct internal failure modes without external intervention. Automation in the fabrication process of smart cells, from sensor integration to pack assembly, where self-healing not only restores performance but also actively maintains the safety condition of operation.

In the long term, the integration of sensing, BMS, and self-healing capabilities will enable the development of smart batteries that continuously monitor, diagnose, and correct internal failure modes without external intervention. A key goal is to advance the concept of self-safety, where self-healing not only restores performance but also actively re-establishes safe operating conditions. Equally important, continuous sensing generates large amounts of valuable data over the entire lifetime of the battery. This “battery life story” provides crucial insights for accurately assessing the state-of-health at end-of-life, supporting second-life applications, informing efficient recycling strategies, and providing a trusted data foundation for the battery passport.

The Future of Battery Sensing Technology

The development of smart functionalities in battery sensing technology is not merely an incremental research step—it is rapidly becoming a defining factor for the next generation of batteries. Future energy storage systems are expected to be long-lasting, more reliable, and capable of continuous communication with their operating environment.

In the next phase of this Roadmap, the priorities must be integration, scalability, and intelligent data management. Sensors should be adaptable to different cell formats and manufacturable through industrial-scale processes. The ultimate goal is to merge sensors, self-healing materials, and the BMS into a coherent, fully functional unit, validated under real-world operating conditions to ensure robustness and efficiency.

A further challenge lies in managing the vast volumes of data generated by these sensors. Robust data management platforms and AI-driven algorithms will be essential to enable real-time monitoring, efficient storage, and predictive analytics, ideally through on-board computation. Achieving this will require overcoming the complexity of lithium battery systems while ensuring reliability, safety, and cost-effectiveness.

Progress will depend on close collaboration between research institutions, industry, and policymakers. Only through coordinated effort can the vision of a safer, smarter, and more sustainable battery future be realised. The next steps will be decisive in bringing that vision from concept to reality.

3.2 Integration of smart functionalities: Self-healing

The transition to clean energy and emission-free mobility demands advanced, sustainable rechargeable batteries with enhanced quality, reliability, lifetime, and safety (QRLS)[173]. Integration of sensing capabilities to detect irreversible damage in batteries was proposed as one of the paths towards the next generation of battery technology[174]. However, to truly enhance QRLS, batteries must not only detect issues arising during cycling but also be capable of restoring their original function through self-repairing mechanisms[175]. This involves preventive strategies addressing degradation during operating conditions and curative actions such as self-healing. Originally inspired by biological systems, self-healing functionalities are explored by researchers for implementation in various battery components—separators, binders, and current collectors[176]. To be useful, self-healing must be tailored to the specific battery chemistry and function of each component. Akin to targeted drug delivery in medicine[177], self-healing could be used to repair damaged electrodes where self-healing agents are delivered on demand inside a battery[178]. This approach is still in its infancy but represents a significant frontier in battery research.

3.2.1 Current Status

Self-healing mechanisms in batteries are classified as either active (requiring no external trigger), or passive, which need a stimulus such as heat, light, or pH changes[179]. To enable rapid and effective repair, self-healing should be directed by highly reactive components. Due to a wide variety of degradation mechanisms in LIBs, many different self-healing approaches have emerged, targeting different degradation mechanisms in batteries. Figure 8 outlines key degradation routes, where each of them presents both challenges and opportunities for self-healing innovation. However, the interaction of battery components is complex, where aging and thus degradation processes are intertwined[180]. The implementation of self-healing functionality as a component can introduce new complex interactions and degradation processes.

[173] Tarascon, J.M., Armand, M., Issues and challenges facing rechargeable lithium batteries. *Nature.* **414** (6861), 359–367, 10.1038/35104644 (2001).
[174] Narayan, R., Laberty-Robert, C., Pelta, J., Tarascon, J.-M., Dominko, R., Self-Healing: An Emerging Technology for Next-Generation Smart Batteries. *Advanced Energy Materials*, 2102652, 10.1002/aenm.202102652 (2021).
[175] BloombergNEF, A Behind the Scenes Take on Lithium-ion Battery Prices (2023), https://about.bnef.com/insights/clean-energy/lithium-ion-battery-pack-prices-hit-record-low-of-139-kwh/.
[176] Narayan, R., Laberty-Robert, C., Pelta, J., Tarascon, J.-M., Dominko, R., Self-Healing: An Emerging Technology for Next-Generation Smart Batteries. *Advanced Energy Materials*, 2102652, 10.1002/aenm.202102652 (2021).
[177] Griffith, L.G., Naughton, G., Tissue engineering--current challenges and expanding opportunities. *Science.* **295** (5557), 1009–1014, 10.1126/science.1069210 (2002).
[178] Guo, K. *et al.,* Smart supercapacitors with deformable and healable functions. *Journal of Materials Chemistry A.* **5** (1), 16–30, 10.1039/C6TA08458C (2017).
[179] Bergman, S.D., Wudl, F., Mendable polymers. *J. Mater. Chem.* **18** (1), 41–62, 10.1039/B713953P (2008).
[180] Narayan, R., Laberty-Robert, C., Pelta, J., Tarascon, J.-M., Dominko, R., Self-Healing: An Emerging Technology for Next-Generation Smart Batteries. *Advanced Energy Materials*, 2102652, 10.1002/aenm.202102652 (2021).

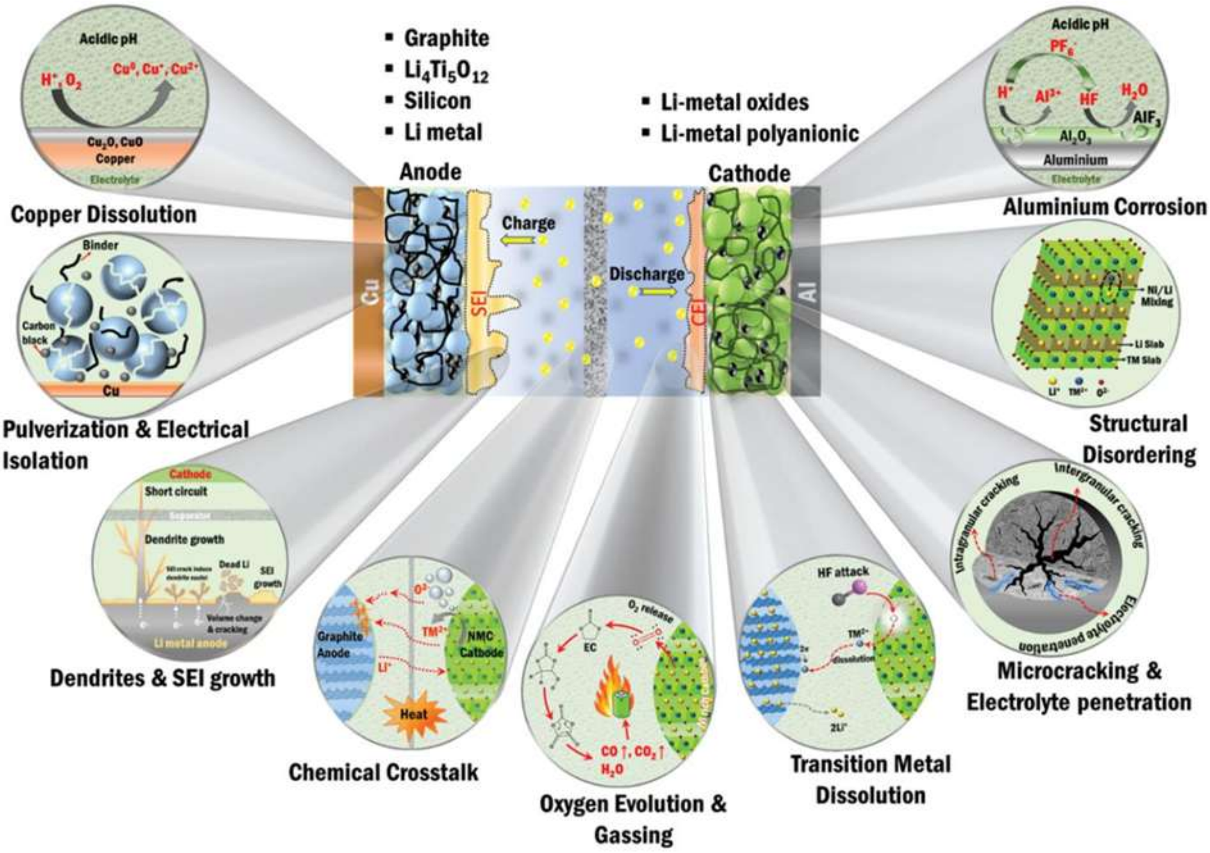

FIGURE 8. Overview of the major degradation mechanisms in the Li-ion batteries.

Self-healing strategies

Self-healing activities within the field of batteries have mainly targeted the self-repair of electrodes, as well as functionalized membranes to regulate ion transport or minimise parasitic reactions. Some of these aspects (divided according to functionality) are addressed in more detail below.

Restoration of electrode conductivity

Maintaining electrical properties of components is crucial in energy storage devices. One promising self-healing approach uses microcapsules containing releasable conductive materials to re-establish physical and electrical integrity at damaged sites. Early studies employed urea-formaldehyde microcapsules filled with carbon nanotubes (CNTs) in solvents such as chlorobenzene, enabling both mechanical and conductive healing. When embedded in epoxy and then fractured, these capsules burst, releasing CNTs that restore conductivity in cracked gold lines within minutes, demonstrating the potential of self-healing conductive systems (see Figure 9)[181].

[181] Odom, S.A. *et al.,* Autonomic restoration of electrical conductivity using polymer-stabilized carbon nanotube and graphene microcapsules. *Applied Physics Letters.* **101** (4), 43106, 10.1063/1.4737935 (2012).

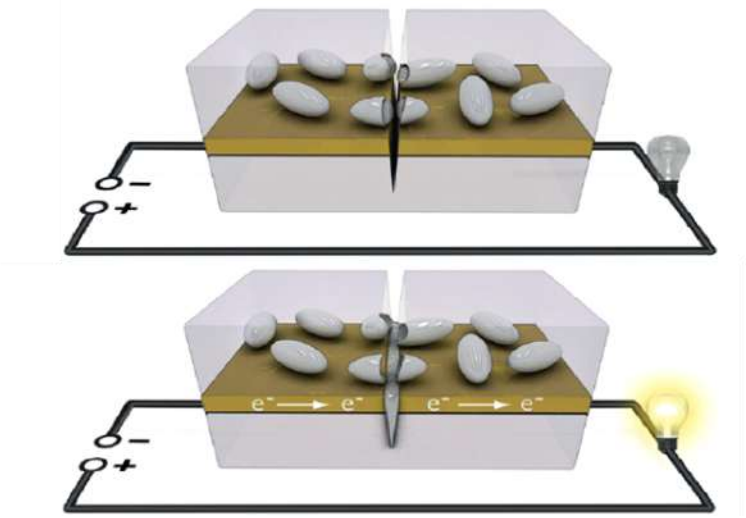

FIGURE 9. Testing self-healing of the gold line after damage.

Other conductive systems, such as carbon-black (CB) dispersions, have been encapsulated and tested due to the use of CB in existing graphite anodes[182,183]. When combined with poly-(3-hexylthiophene) (P3HT), these dispersions helped to restore conductivity in cracked silicon (Si) anodes, which suffer from significant volume changes during lithiation. However, the approach is irreversible and reduces energy density due to inactive microcapsules.

Functionalized separators

Within the development and optimization of battery chemistry, the primary focus is typically devoted to active materials and electrolytes while modification of separators is generally overlooked. During battery operation, redox reactions often cause unwanted side reactions at unstable interfaces, releasing degradation products such as dissolved metals or organic compounds. These can pass through a separator, deposit on electrodes, or cause self-discharge. To prevent this, separators could be functionalized with chelating agents to capture metal ions or grafted with proteins to control the movement of harmful organic species.

Using separators to anchor trapping molecules within their porous structure offers several advantages:

- dissolved transition metal ions migrate through the separator, making them accessible for capture; the separator's high porosity provides a large surface area for effective trap distribution and ion capture;
- traps are positioned away from electrochemical reaction zones, protecting their stability;
- separators serve as a suitable platform for ion uptake at room temperature; and
- they can be engineered with self-healing properties.

Cyclodextrins are promising for separator functionalization due to their solubility, biocompatibility, and ability to form inclusion complexes with small molecules or cations. Their temperature-dependent trapping behaviour also allows for controlled uptake and release. Alternatives like crown ethers and calixarenes offer open structures for anchoring chelating ligands to regulate ion transport, though they are less environmentally friendly. These materials are relatively easy to graft, making them attractive for developing smart, responsive battery separators.

Designing electrolytes with self-healing functionalities

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[182] Blaiszik, B.J., Jones, A.R., Sottos, N.R., White, S.R., Microencapsulation of gallium-indium (Ga-In) liquid metal for self-healing applications. *Journal of Microencapsulation.* **31** (4), 350–354, 10.3109/02652048.2013.858790 (2014).

[183] Kang, S., Jones, A.R., Moore, J.S., White, S.R., Sottos, N.R., Microencapsulated Carbon Black Suspensions for Restoration of Electrical Conductivity. *Advanced Functional Materials.* **24** (20), 2947–2956, 10.1002/adfm.201303427 (2014).

Self-healing electrolytes offer a promising strategy to enhance performance and durability in both aqueous and non-aqueous batteries. In Li-sulfur (Li-S) batteries, a self-healing electrolyte was developed to counter polysulfide shuttling by maintaining a dynamic equilibrium at the sulfur/electrolyte interface, achieving 1450 mAh g^{-1} capacity and high coulombic efficiency[184]. Peng et al. further improved this chemistry with self-healing electrolytes containing auto-repairing agents that mimic biological fibrinolysis and dissolve solid Li_2S thus enabling over 2000 stable cycles[185]. Self-healing functionalities have also been incorporated into polymerizable ionic liquid (PIL) electrolytes[186]. These PILs support the development of flexible and wearable electronics, though challenges remain, including low ionic conductivity and high interfacial resistance—often requiring high temperatures or prewetting to operate[187,188, 189].

Additionally, battery performance depends on the choice of separator material, impacting overall sustainability[190]. In aqueous Zn-ion batteries (ZIBs), Huang et al. developed a hydrogel electrolyte using a freeze/thaw method with PVA/$Zn(CF_3SO_3)_2$, which self-heals via hydrogen bonding[191]. This hydrogel incorporates all battery components and enables full performance recovery after multiple damage-healing cycles. Such developments open new possibilities for sustainable, self-healing energy storage devices, particularly in flexible and wearable technologies.

Other self-healing strategies

Self-healing can involve many kinds of bonding, such as supramolecular interactions, which frequently involve Hydrogen (H) bonding. However, this is not ideal for the design of self-healing binders for non-aqueous battery systems due to parasitic reactions involving hydroxyl groups. In aqueous systems, though, Zhao et al. showed that flexible, self-healing aqueous Li-ion batteries could be created using aligned CNT sheets and healing polymer substrates[192]. Once cut, these batteries self-repaired within seconds. Similarly, Xie et al. introduced a self-healing zinc-iodine flow battery where a porous membrane absorbs I_3^- and enables dendrite oxidation and recovery during overcharging[193]. Wang's group developed hydrogen-bonding polymer coatings and later 3D-distributed self-healing polymers,

[184] 248. Xu, R. *et al.,* Role of Polysulfides in Self-Healing Lithium-Sulfur Batteries. *Advanced Energy Materials.* **3** (7), 833–838, 10.1002/aenm.201200990 (2013).
[185] Peng, H.-J. *et al.,* Healing High-Loading Sulfur Electrodes with Unprecedented Long Cycling Life: Spatial Heterogeneity Control. *Journal of the American Chemical Society.* **139** (25), 8458–8466, 10.1021/jacs.6b12358 (2017).
[186] Eftekhari, A., Saito, T., Synthesis and properties of polymerized ionic liquids. *European Polymer Journal.* **90**, 245–272, 10.1016/j.eurpolymj.2017.03.033 (2017).
[187] Tian, X. *et al.,* Self-healing and high stretchable polymer electrolytes based on ionic bonds with high conductivity for lithium batteries. *Journal of Power Sources.* **450**, 227629, 10.1016/j.jpowsour.2019.227629 (2020).
[188] Chen, W. *et al.,* A Self-Healing Ionic Liquid-Based Ionically Cross-Linked Gel Polymer Electrolyte for Electrochromic Devices. *Polymers.* **13** (5), 10.3390/polym13050742 (2021).
[189] Safa, M., Chamaani, A., Chawla, N., El-Zahab, B., Polymeric Ionic Liquid Gel Electrolyte for Room Temperature Lithium Battery Applications. *Electrochimica Acta.* **213**, 587–593, 10.1016/j.electacta.2016.07.118 (2016).
[190] Eftekharnia, M., Hasanpoor, M., Forsyth, M., Kerr, R., Howlett, P.C., Toward Practical Li Metal Batteries: Importance of Separator Compatibility Using Ionic Liquid Electrolytes. *ACS Applied Energy Materials.* **2** (9), 6655–6663, 10.1021/acsaem.9b01175 (2019).
[191] Huang, S. *et al.,* A Self-Healing Integrated All-in-One Zinc-Ion Battery. *Angewandte Chemie International Edition.* **58** (13), 4313–4317, 10.1002/anie.201814653 (2019).
[192] Zhao, Y. *et al.,* A Self-Healing Aqueous Lithium-Ion Battery. *Angewandte Chemie International Edition.* **55** (46), 14384–14388, 10.1002/anie.201607951 (2016).
[193] Xie, C., Zhang, H., Xu, W., Wang, W., Li, X., A Long Cycle Life, Self-Healing Zinc-Iodine Flow Battery with High Power Density. *Angewandte Chemie International Edition.* **57** (35), 11171–11176, 10.1002/anie.201803122 (2018).

improving mechanical resilience and cycling stability[194,195,196,197] (Figure 10). Other supramolecular binders have also been explored, though long-term testing remains essential for practical evaluation[198,199,200,201,202,203].

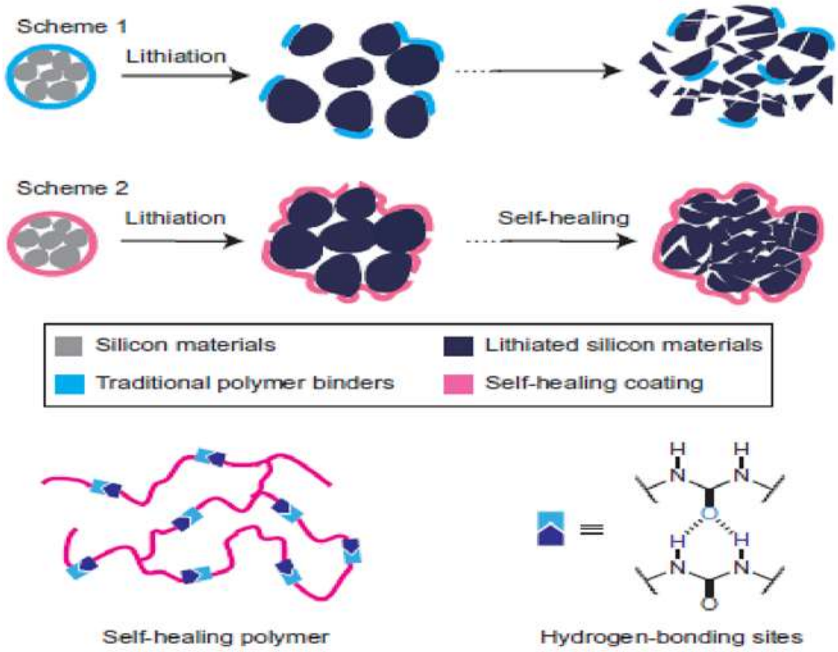

FIGURE 10. Design and structure of a self-healing silicon electrode.

Jin et al. developed a self-healing system using a TiO_2@Si yolk–shell structure with both artificial and natural SEI. During lithiation, Silicon (Si) expansion expelled the internal electrolyte, exposing the Si core to the TiO_2 shell and forming fresh SEI layers that bridged cracks. This design achieved over 99.9% coulombic efficiency and excellent cycling stability[204].

Dendrite growth is a major challenge in non-aqueous and solid-state Li metal batteries. Li et al. applied high plating/stripping currents (~9 mA cm^{-2}) to induce surface Li migration that smoothed the metal

[194] Kwon, T., Choi, J.W., Coskun, A., Prospect for Supramolecular Chemistry in High-Energy-Density Rechargeable Batteries. *Joule.* **3** (3), 662–682, 10.1016/j.joule.2019.01.006 (2019).
[195] Wang, C. *et al.,* Self-healing chemistry enables the stable operation of silicon microparticle anodes for high-energy lithium-ion batteries. *Nature Chemistry.* **5** (12), 1042–1048, 10.1038/nchem.1802 (2013).
[196] Tee, B.C.-K., Wang, C., Allen, R., Bao, Z., An electrically and mechanically self-healing composite with pressure- and flexion-sensitive properties for electronic skin applications. *Nature Nanotechnology.* **7** (12), 825–832, 10.1038/nnano.2012.192 (2012).
[197] Chen, Z. *et al.,* High-Areal-Capacity Silicon Electrodes with Low-Cost Silicon Particles Based on Spatial Control of Self-Healing Binder. *Advanced Energy Materials.* **5** (8), 1401826, 10.1002/aenm.201401826 (2015).
[198] Jeong, Y.K. *et al.,* Hyperbranched β-cyclodextrin polymer as an effective multidimensional binder for silicon anodes in lithium rechargeable batteries. *Nano letters.* **14** (2), 864–870, 10.1021/nl404237j (2014).
[199] Kwon, T. *et al.,* Dynamic Cross-Linking of Polymeric Binders Based on Host-Guest Interactions for Silicon Anodes in Lithium-Ion Batteries. *ACS nano.* **9** (11), 11317–11324, 10.1021/acsnano.5b05030 (2015).
[200] Kang, S., Yang, K., White, S.R., Sottos, N.R., Silicon Composite Electrodes with Dynamic Ionic Bonding. *Advanced Energy Materials.* **7** (17), 1700045, 10.1002/aenm.201700045 (2017).
[201] Munaoka, T. *et al.,* Ionically Conductive Self-Healing Binder for Low-Cost Si Microparticles Anodes in Li-Ion Batteries. *Advanced Energy Materials.* **8** (14), 1703138, 10.1002/aenm.201703138 (2018).
[202] Kwon, T. *et al.,* Systematic molecular-level design of binders incorporating Meldrum's acid for silicon anodes in lithium rechargeable batteries. *Advanced Materials.* **26** (47), 7979–7985, 10.1002/adma.201402950 (2014).
[203] Zeng, F. *et al.,* Multidimensional Polycation β-Cyclodextrin Polymer as an Effective Aqueous Binder for High Sulfur Loading Cathode in Lithium-Sulfur Batteries. *ACS applied materials & interfaces.* **7** (47), 26257–26265, 10.1021/acsami.5b08537 (2015).
[204] Jin, Y. *et al.,* Self-healing SEI enables full-cell cycling of a silicon-majority anode with a coulombic efficiency exceeding 99.9%. *Energy & Environmental Science.* **10** (2), 580–592, 10.1039/C6EE02685K (2017).

surface and enabled uniform current distribution, effectively suppressing dendrite formation. Repeated high-current pulses allowed Li–S batteries with 0.1 M $LiNO_3$ to cycle with high efficiency. Other self-healing strategies for countering dendrite formation use additives; for instance, Ding et al. employed a self-healing electrostatic shield by Cs^+ and Rb^+ additives[205].

Another self-healing strategy involves liquid metal anodes which undergo reversible liquid–solid–liquid transitions during cycling, as demonstrated by Deshpande et al. with Lithium–Gallium (Li_2Ga) alloy[206]. This property enables healing of micro-cracks formed during lithiation/delithiation. Such a concept has been further extended to other alloying active materials and battery chemistries, including Ga-Sn electrodes, which demonstrated over 4000 cycles and stable capacity[207], and Sodium–Tin alloys (Na-Sn) alloys for Na-ion batteries[208]. Other self-healing advancements include thermo-switchable polymers for thermal self-protection and integration of self-healing features into electrolytes and current collectors[209].

In the European landscape, a conductive and self-healing polymer binder was developed for the BAT4EVER project. This polymer was implemented in the silicon anode, supporting the electrode's conductivity with its own conductivity and preserving the electrode's structure despite silicon's volume expansion through its self-healing property.

Within the SALAMANDER project, novel self-healing polymers are being developed and tested in Si anodes to improve stability during cycling and repair cracks that form during anode degradation[210]. The thermally triggered self-healing mechanism is complemented by the development of a printed sensor designed to monitor the anode layer's resistance and thereby detect cracking phenomena. In conclusion, the field of BSH is rapidly gaining momentum as a part of smart battery design.

3.2.2 Challenges

Self-healing as active function in battery environment

Passive self-healing capabilities are too limited to target the whole spectrum of battery degradation mechanisms. Rather than simply embedding passive materials with self-healing functionality, the long-term challenge is to activate healing in response to specific degradation signatures triggered via sensing and governed by BMS to initiate the healing process. Integration and optimization of sensors and BMS are challenges that are addressed in Chapter 3.1.1 *Sensing*. For that purpose, the type of trigger and self-healing mechanism needs to be carefully designed and chemically interconnected to be defined as a closed loop system.

The choice of stimulus or actuation to activate self-healing may lead to side effects and unintended consequences for non-self-healing components. For example, if an increase in temperature is needed for healing, it may also lead to the premature or accelerated decomposition of electrolyte. A magnetic field may activate self-healing but interfere with the electric field between electrodes. It may be challenging for a stimulus to only target the self-healing component and not influence in some way other components, particularly if the actuator is external to the cell while the self-healing component is embedded in the cell. The effects from stimuli like temperature, pressure, or optical light might be

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[205] Ding, F. *et al.,* Dendrite-free lithium deposition via self-healing electrostatic shield mechanism. *Journal of the American Chemical Society.* **135** (11), 4450–4456, 10.1021/ja312241y (2013).
[206] Deshpande, R.D., Li, J., Cheng, Y.-T., Verbrugge, M.W., Liquid Metal Alloys as Self-Healing Negative Electrodes for Lithium-Ion Batteries. *Journal of The Electrochemical Society.* **158** (8), A845, 10.1149/1.3591094 (2011).
[207] Wu, Y. *et al.,* A room-temperature liquid metal-based self-healing anode for lithium-ion batteries with an ultra-long cycle life. *Energy & Environmental Science.* **10** (8), 1854–1861, 10.1039/C7EE01798G (2017).
[208] Mao, J., Fan, X., Luo, C., Wang, C., Building Self-Healing Alloy Architecture for Stable Sodium-Ion Battery Anodes: A Case Study of Tin Anode Materials. *ACS applied materials & interfaces.* **8** (11), 7147–7155, 10.1021/acsami.6b00641 (2016).
[209] Kelly, J.C., Gupta, R., Roberts, M.E., Responsive electrolytes that inhibit electrochemical energy conversion at elevated temperatures. *Journal of Materials Chemistry A.* **3** (7), 4026–4034, 10.1039/C4TA06482H (2015).
[210] https://www.salamander-eu.com/

well known, but others like acoustic or magnetic fields could be much less understood, especially for slow-acting, long-term degradation mechanisms.

Self-healing strategies are partially hindered by their inherent complexity, as any self-repairing chemistry must also withstand the cell's harsh oxidizing and reducing environment. This challenge includes not only the interactions with the electrolyte, but also factors such as the voltage window and temperature fluctuations during cycling. To address these issues, researchers have developed polymers with intrinsic self-healing properties leveraging dynamic supramolecular interactions, such as hydrogen bonding, electrostatic crosslinking and host–guest chemistry, and Van der Waals forces[211]. Another self-healing strategy involves functionalized polymers that are compatible with battery components and respond to damage by producing reactive species. However, incorporating self-healing polymers or ionic liquids into electrolyte systems can be challenging in cell design, as they may alter interface chemistry and layer thickness. Despite these challenges, this field is quickly evolving, with recent studies demonstrating progress in integrating self-healing functionalities into batteries and supercapacitors[212].

Definitions and standardization

The ongoing debate that should be solved in the battery community is how to define and measure self-healing within batteries. The original concept of self-healing as defined in nature or other disciplines is not directly translatable to the working concept of self-healing functionalities in a battery. An example is the use of self-healing polymers as binder materials in electrodes. The self-healing properties of polymers are typically evaluated in pure polymer films, by testing the ability to repair a micro-sized cut in the film, either with or without external trigger. However, in batteries, only a small percentage (up to a few wt-%) of an electrode consists of binder (especially in industrial settings), which may impede self-healing abilities. Although many binders with self-healing capabilities described in literature are shown to improve either the capacity or lifetime of battery (generally tested in half or full cell coin cells), typically no direct proof of healing (e.g., improved performance due to an external trigger) is provided. Further proof of self-healing could be chemical evidence of reversible chemical interactions between self-healing groups in a polymer as a function of cycling. Hence, there is a strong need for the development of testing matrices, standard metrics and testing procedures, and characterization tools as well as a general agreement on the definition of self-healing.

Manufacturability, circularity, scalability and reliability

Self-healing capability is a promising but challenging addition to next-generation batteries. It can provide significant performance advantages, particularly for premium markets and high-stress applications, but at the expense of increased complexity and possibly decreased recyclability if not properly designed. Therefore, innovations in affordable, scalable, and recyclable self-healing materials are crucial for broad implementation. The addition of self-healing functionality complicates production in terms of material synthesis, integration and quality control. The preparation of self-healing materials or components (for example, microcapsules or dynamic covalent networks) often require complicated chemical synthesis or mixing techniques. Furthermore, the incorporation of self-healing components may necessitate the inclusion of additional production procedures such as coating, curing, or encapsulating while their compatibility and stability in such processes is unknown. It also might be necessary to use new inspection techniques in quality control to confirm the distribution and functionality of curative agents. This manufacturing complexity makes the implementation of self-healing materials in scalable production lines rather difficult.

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[211] Wang, H. *et al.,* Recent Advances on Self-Healing Materials and Batteries. *ChemElectroChem.* **6** (6), 1605–1622, 10.1002/celc.201801612 (2019).

[212] Cheng, Y., Xiao, X., Pan, K., Pang, H., Development and application of self-healing materials in smart batteries and supercapacitors. *Chemical Engineering Journal.* **380**, 122565, 10.1016/j.cej.2019.122565 (2020).

The inverse challenge of stability is that some self-healing components may be inherently unstable or metastable. For example, consider a reactive Li salt in a degradable encapsulation; under the intended stimulus in the cell, the encapsulation degrades and additional ions are released, extending the cell life time. However, in the time before it is integrated into the manufacturing process, it may pose a significant safety risk if the encapsulation material degrades before intended, for example during other storage or manufacturing steps. Integration into an electrode or cell/system component may cause that component to be substantially more hazardous than previously considered.

Due to complexities mentioned above, material, process and end-product costs for batteries with self-healing functionalities are expected to be higher than those for conventional batteries. In terms of material cost, self-healing materials and components tend to be more expensive than conventional materials in the unit cell. The synthesis costs of these materials and components are also high, both in terms of raw materials and processes. Thus, the additional steps in synthesizing and implementing these materials and components will increase CAPEX and OPEX. However, thanks to the prolonged cycle life of self-healing batteries, there is still a potential to reach competitive costs per kWh per cycle delivered.

Self-healing materials and components could also potentially have challenges in terms of recyclability. These materials and components are more complex than conventional materials and may require more sophisticated systems to separate and recycle them. They may also exhibit unexpected behaviour during separation and recycling and may cause the need to alter this process. However, self-healing materials and components are expected to provide lifecycle benefits as extended lifetime reduces the number of times batteries are replaced and total lifecycle waste is reduced. Altogether, thorough life cycle assessment (LCA) is still necessary to determine the value of self-healing functionalities in batteries.

Despite promising advances in the development of self-healing functionalities for batteries, significant challenges remain. Most current demonstrations are limited to laboratory scale research and have yet to be translated into real-world applications. Bridging the gap between fundamental research and practical implementation requires not only further technological innovation but also the development of scalable, robust strategies. Overcoming these hurdles is essential to fully realize the performance and reliability benefits that self-healing batteries can offer.

3.2.3 Advances needed to meet the challenges

Common language, definition, and testing protocol around self-healing

As identified earlier, self-healing lacks consistency in definition, terminology, and testing protocols. Standard operating procedures should be developed, initially for the most well understood self-healing functionalities; these should be digitally ontologized and shared in the robust data, education, and standards framework being developed by Battery 2030+. Several discussions and forums for the self-healing community to gather and debate on some agreed terms will become necessary in the future for the field to advance more quickly and make better use of the research being conducted.

Standardization

A critical challenge in the battery community is establishing a clear and universally accepted definition of self-healing in batteries. To advance the field, there is a strong need for the development of standardized testing protocols, metrics, and characterization tools, as well as community consensus on the definition and measurable criteria of self-healing in practical battery systems.

Self-healing electrodes

There is a need for materials and systems that can actively restore electrical connectivity following electrode damage. This includes the development of sliding gels with reversible bonds that can reorganize at the surface and absorb mechanical stress via a “pulley effect” along polymer chains. Such materials must be optimized to not only facilitate self-healing but also provide mechanical reinforcement. Additionally, there is a need for composite electrodes incorporating microcapsules capable of targeted, on-demand release of healing agents. These capsules should be engineered with robust shell materials and contain compounds such as Li(Na)-based sacrificial salts or other active substances to enable precise and efficient repair. Furthermore, an important approach to compensate for the loss of active lithium due to SEI formation involves incorporating thermally triggerable microvesicles containing Li-salts into the cathode. These microvesicles can act as a supplementary lithium-ion source, releasing lithium on demand to maintain cell performance. Both microcapsules and microvesicles require a clear understanding of how to synthesize and control their trigger mechanism precisely; the tunability thereof is important for enabling broader uptake in other battery systems.

Polymer membranes

Polymer membranes are key to developing self-healing batteries, serving as solid polymer electrolytes, redox-active electrode materials, and components of hybrid systems. Their ability to form or cross-link in situ enables them to act as mechanical healing agents, similar to resins like epoxy. Polymers can also template inorganic capsule formation and support virtually limitless composite applications. Supramolecular assembly, particularly hydrogen bonding, offers short-term solutions for stabilizing electrolytes and enabling conductive, self-healing materials. Other approaches include metal-ion complexation in ionomers, reversible S–S covalent bonding, and multiphasic solid polymer systems that respond to stimuli for healing. As such, they are central to Battery 2030+ self-healing strategies.

Bio-sourced membranes

Developing methods that replicate the selective barrier properties of biological membranes is crucial for controlling electrolyte decomposition and enhancing the battery ageing. A key milestone will be to monitor, inside the battery, electrolyte stability using a sensitive and selective sensor at the single-molecule scale using nanopore technology with electrical detection. For this to happen, one must design thin and porous controlled membranes using the chemistry of non-toxic and bio-sourced molecules/proteins (e.g., cyclodextrins) whose selectivity can be achieved by the use and optimisation of protein engineering.

Integration into existing and forthcoming manufacturing and recycling processes

For the most rapid deployment of self-healing functionalities into existing battery chemistries, the materials and components should be compatible with as much existing manufacturing equipment as possible. To overcome this challenge, self-healing materials and components must be developed to higher TRLs and produced in larger quantities that can be tested on pilot-scale manufacturing lines. Earlier input from cell manufacturers and similar stakeholders in the advancement of self-healing materials and components is necessary to accelerate their adoption. However, new manufacturing processes are also forthcoming, such as dry electrode coating or solid-state battery assembly. Significant effort is necessary for self-healing materials and components to be adapted to these newer processes and to understand their impact on downstream processes. Likewise, gathering input and understanding the future progression of battery recyclers and their processes can help drive the design of self-healing materials towards successfully recyclable components.

Quantifying the impact of self-healing functionalities

Presently, self-healing in batteries is an ambitious and promising concept, but its actual quantified impact on QRLS, for example, is still in its infancy. An LCA study of a self-healing battery published in 2025 is claimed to be the first of its kind[213]. More analyses for various types of self-healing materials and components will be needed to quantify the cost vs. benefit between building a smart self-healing battery and replacing a conventional battery. These analyses also inherently depend on research and

[213] Philippot M.L. *et al.*, Healing the battery and the planet: An environmental perspective on self-healing batteries for smartphones, *Journal of Cleaner Production*. **489**, 2024.144645, 2025.

performance data on self-healing batteries. At its best, conducting LCA during the development of self-healing materials and components may help select the best candidates for eventual implementation.

3.2.4 Forward vision

Addressing battery degradation requires a multidisciplinary approach, combining intrinsic and extrinsic self-healing tailored to specific chemistries. Inactive components such as separators or binders can store microcapsules with sacrificial salts or additives to restore Li concentration or dissolve passive films. These extrinsic systems should respond to triggers like temperature, pressure, or volume changes. Successful on-demand healing depends on integrating sensing and self-healing, a key goal of Battery 2030+, enabling targeted, *in vivo*-like interventions in batteries.

Battery sustainability can be enhanced by integrating bio-sourced materials with self-healing functionalities. Proteins, polysaccharides, and polyesters offer potential for modifying components to enable cation transport, electrode integrity, and degradation product capture. Natural polymers can be tailored for these roles. However, replicating biological membrane selectivity and monitoring electrolyte stability with biomimetic sensors remain challenging. Functionalizing macrocyclic cages like cyclodextrins or calixarenes on polyethylene terephthalate (PET) separators may help capture parasitic redox species and improve battery performance.

To fully benefit from self-healing functionalities, battery research must focus on optimizing self-healing kinetics. Addressing this requires bold, open-minded approaches while considering key constraints like performance goals, chemical environment, and manufacturing compatibility.

European research on BSH is advancing, with growing industry interest and emerging expertise that could position Europe as a global leader. Despite the low TRL, the Battery 2030+ programme aims to translate lab-scale progress into impactful innovations through a strong IPR and commercialization strategy. Its ambitious BSH roadmap seeks to enhance battery QRLS and unite a multidisciplinary community toward the shared goal of developing durable, self-healing batteries. Key milestones to achieve this vision are outlined below.

The Safe and Sustainable by Design (SSbD) framework marks a major step forward for battery innovation, but it currently does not fully address the recyclability of battery components. Many battery materials and components are already technologically mature, making it increasingly difficult to retrofit or redesign them for efficient recycling. Meanwhile, self-healable components are still in the early stages of development and have yet to be widely adopted. This gap highlights a significant opportunity: by evolving the SSbD framework to Safe, Sustainable and Recyclable by Design (SSRbD) framework. Such an expanded approach would encourage the design of batteries that are not only safer and more sustainable, but also easier to recycle, supporting a true cradle-to-cradle lifecycle.

In the short-term (2025–2027): It is important to establish a common vocabulary and metrics for smart functionalities, sensing, and self-healing. Validating the accuracy and reproducibility of self-healing stimuli or actuator mechanisms is key for their reliability. Additionally, prototyping modular BMS calibrated with self-healing data is a priority. Efforts should also focus on exploring the physical and economic integration of smart components into manufacturing processes, while standardizing test protocols for assessing self-healing responses.

In the medium-term (2027–2030): The objective is to demonstrate closed-loop systems that combine sensors, self-healing mechanisms, and BMS within scalable battery formats. Establishing robust design guidelines will be essential to ensure that smart functionalities can be integrated without compromising cell integrity or recyclability. In parallel, assessing the total cost of ownership and the added value of smart batteries in strategic applications will be crucial for gauging their practical viability. Importantly, self-healing capabilities should be proven at both pilot and full-scale manufacturing levels.

Self-healing components should demonstrate chemistry agnosticism—that is, the ability to function effectively across different cell chemistries with minimal adjustment or intervention. Beyond Generation 3 Li-ion systems, the principles of self-healing should also be validated and progressively tailored to address degradation mechanisms in other metal-ion and solid-state chemistries.

In the long-term (2030 and beyond): The objective is to enable fully self-aware batteries that can continuously monitor, diagnose, and correct internal failure modes autonomously. Integrating smart functionalities with digital twins, manufacturing systems, and recycling pathways will support sustainable battery life cycles. The development of industry-ready smart cell formats featuring embedded diagnostics and feedback control is essential for commercialization.

To ensure market acceptance and widespread adoption, regulatory and safety frameworks for active battery systems must be defined, alongside advocacy for the inclusion of smart functionalities as standard criteria in future sustainable battery certifications. In this vision, self-healing becomes an inherent aspect of the battery lifetime, enabling a true understanding of real-world durability in commercial applications. Sensors and predictive models will not only detect damage but also quantify the remaining self-healing capacity. Research and development will push towards batteries with indefinite—or near-indefinite—lifetimes, achievable through simple maintenance procedures. Self-healing mechanisms will be designed to be fully recyclable and/or reusable.

4.NEW BATTERY CHEMISTRIES AND NEW TECHNOLOGIES

The development of new battery chemistries is critical to meeting the ambitious sustainability and strategic goals outlined in the B2030+ roadmap. Traditional lithium-ion technologies, while progressing rapidly, have inherent limitations in terms of cost, sustainability and resource availability. Emerging chemistries present an opportunity to overcome these barriers, offering alternative pathways toward high-performance, safe and sustainable energy storage solutions.

In this context, the exploration of post-lithium technologies is not just a scientific pursuit but a strategic necessity. Emerging chemistries offer the potential to diversify the European battery landscape, reducing dependency on critical raw materials, and enabling applications that are not achievable with current technologies, such as long-duration storage and high-energy mobile applications. Integrating them into the broader Battery 2030+ strategy ensures alignment with EU sustainability goals and energy system decarbonization.

4.1 Introduction

The search for new battery chemistries and technologies remains one of the most dynamic yet fragmented areas of battery research. In recent years, several new battery chemistries have been proposed, many still within LIBs domain, such as disordered rock salts (DRX) which are attracting attention for their high capacity and structural versatility. Parallel progress has been made on lithium manganese iron phosphate (LMFP), lithium nickel manganese oxide (LNMO) and lithium-rich manganese oxide (LRMO). Together, these developments reflect a broader push toward more sustainable, cost-effective, and high-performance alternatives to conventional cathode materials.

Beyond incremental improvements in lithium-ion technology, a diverse landscape of new battery technologies has also emerged over the last decade. Many of these technologies promise significant improvements in cost, safety, sustainability and/or performance. Yet, most remain at low technology readiness levels (TRL < 4) and face major challenges related to stability, scalability, and manufacturability.

Hence, Battery 2030+ does not treat “new chemistries and new technologies” as a monolithic category, but as a cross-cutting priority affecting nearly all aspects of the battery R&D&I chain—from conceptualization and materials discovery to functional optimization, manufacturing, and recycling.

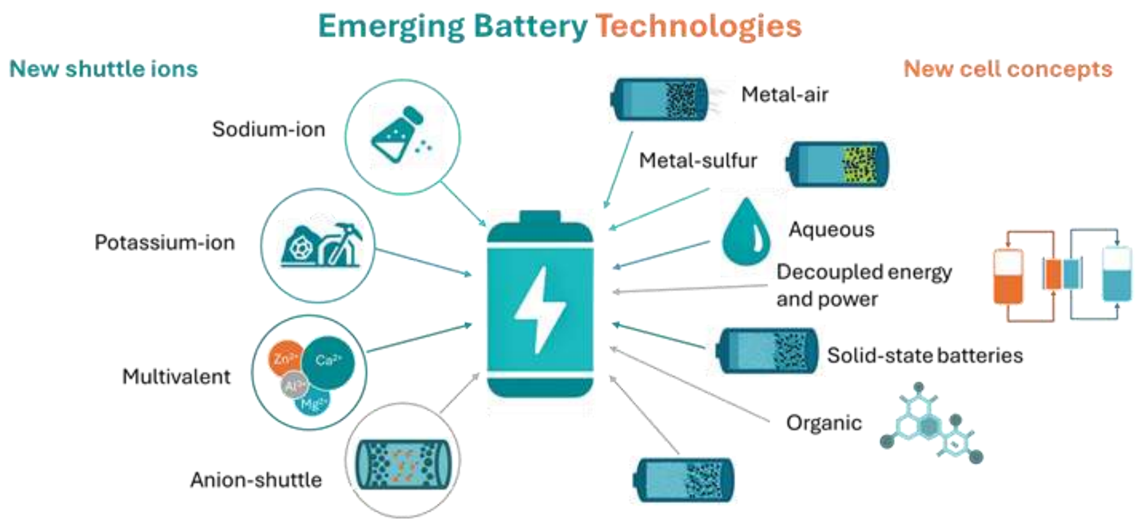

FIGURE 11. NEW CHEMISTRIES AND TECHNOLOGIES, INCLUDING NEW SHUTTLE IONS AND NEW CELL CONCEPTS.

4.2 Current Status

The emerging technologies can be structured into two main categories: (i) new shuttle ions, focusing on the active ion species, and (ii) new cell concepts, which focus on innovative cell architectures applicable across multiple chemistries (see Figure 11).

i) New Shuttle Ions

New shuttle ions refer to the active ion species used in the battery that differ from lithium. Sodium-ion batteries are currently the most mature example, with several chemistries already being tested in pilot-scale production leading to increased efforts and European Commission support focused on improving processability and manufacturability. Potassium-ion batteries, though not yet as advanced, are gaining attention. Magnesium, zinc, calcium and aluminium-based multivalent batteries are also at an earlier stage of development, offering potential advantages in cost, abundance and sustainability, but their progress is limited by fundamental challenges in ion mobility, solvation, and interface stability. Chloride-ion and other anion-shuttle systems offer the advantage to utilize several oxidation states of the involved metals but are still largely at the research stage, with low TRLs and significant scientific and engineering hurdles.

(ii) New Cell Concepts

New cell concepts include technologies that can be applied to various chemistries to enhance energy density, safety or longevity. Examples include metal-air batteries, metal-sulfur batteries, aqueous batteries, organic batteries, solid-state batteries, zero-excess anode concepts and architectures enabling decoupled energy and power (i.e. redox flow batteries). These concepts focus on innovations at the cell level, encompassing not only architecture and materials, but also the fundamental reaction mechanisms and the nature of the active reactants, enabling enhanced energy density, safety, and functionality across different chemistries

Solid-state batteries, for instance, replace the liquid electrolyte with a solid, offering potential safety improvements and enabling higher energy densities. Metal-air batteries offer extremely high theoretical energy densities but face fundamental issues with stability and reversibility. Metal-sulfur batteries provide a low-cost alternative with high capacity, but their cycle life and stability remain limited. Zero-excess anode concepts are being developed to optimize electrode utilization and reduce cost, though they require precise control of plating and stripping mechanisms through interfacial engineering. Hybrid and organic batteries introduce flexibility and tunability in design, combining chemical and structural innovations to address specific application needs.

4.3 Challenges

Despite the breadth of scientific creativity and the large number of projects initiated across Europe, the development of new battery chemistries and technologies is still constrained by a set of persistent and interrelated challenges, spanning from fundamental materials science to large-scale manufacturability. While each technology presents unique obstacles, common issues include stability of electrodes and electrolytes, limited cycle life, low ionic conductivity in some systems and difficulties in scaling laboratory prototypes to commercially relevant formats.

For new shuttle ions, the challenges vary depending on the chemistry and its maturity level. Sodium-ion batteries, although more advanced, require further work on electrolytes and both cathode and anode materials to improve energy density, electrode processability and large-format cell performance. Multivalent-ion systems, such as magnesium, zinc, and aluminium, face limitations in ion mobility, solvation and interface stability, which restrict power density and cycle life. Here, the pathway of the ion must be designed according to the optimal needs of the ion. Early-stage anion-shuttle systems demand breakthroughs in liquid and solid electrolyte design, the application of cathodes with high capacity but with instabilities to become viable.

New cell concepts bring additional challenges that go beyond the choice of the active ion. Technologies such as metal-air, metal-sulphur, aqueous, organic, solid-state and zero-excess anode systems require careful optimization of the reaction mechanisms, electrode/electrolyte interfaces and the overall ionic and electronic conductivity within the cell. Metal-air batteries, for example, face critical issues with passivation, poor reversibility of the oxygen reactions, catalyst degradation and low round-trip efficiency. Metal-sulphur systems are limited by polysulfide shuttling electrode and electrolyte degradation over cycles. Solid-state and zero-excess anode batteries need precise control over plating/stripping processes and interfacial stability. Organic and hybrid systems require materials with improved solubility, electrochemical stability and tuneable redox properties. Challenges specific to decoupled energy/power systems include scaling flow architectures, minimizing crossover and parasitic reactions and ensuring pump efficiency and stability under high cycling rates.

Manufacturing and scale-up represent a critical bottleneck for many emerging chemistries. While some technologies, like sodium-ion, can leverage existing LIB production lines with minimal adaptation, others (including solid-state, metal-air, and metal-sulphur batteries) will require substantial modifications to electrode fabrication, electrolyte integration and cell assembly processes. Developing scalable, cost-effective manufacturing methods is essential to increase the level of maturity. Furthermore, digital twins and advanced modelling are increasingly critical tools, enabling predictive control, real-time monitoring and process optimization across multi-stage manufacturing, from slurry mixing and electrode coating to cell assembly and formation.

Closely linked to manufacturing is the need to design new chemistries and cell architectures with circularity and regulatory requirements in mind. New chemistries must be designed with recyclability, low environmental impact and reduced dependence on critical raw materials, in line with EU regulations such as PFAS restrictions and the CRM strategy. Integrating these considerations from the earliest stages of research ensures that the resulting technologies are not only high-performance but also aligned with Europe's long-term environmental and energy security goals.

Furthermore, advances in embedded sensing technologies and self-healing components should be leveraged to support new chemistries, enabling real-time monitoring, degradation management and predictive optimization of battery performance and lifetime. At the same time, their integration in new chemistries introduces additional constraints: materials must be chemically compatible with embedded sensors and allow reliable signal acquisition, while self-healing mechanisms need to be adapted and optimized for each new chemistry and cell architecture.

Finally, beyond technical hurdles, strategic challenges also exist. Many of these chemistries are still confined to laboratory-scale research and European efforts remain fragmented, which limits visibility and slows progress. Industrial interest in high-risk, high-reward chemistries is often low due to perceived uncertainties. The current Horizon Europe project structure, with long project cycles and rigid KPIs, is frequently ill-suited for accelerating TRLs or enabling rapid iteration of novel chemistries. There is an opportunity to redefine project typology to provide more flexibility, such as establishing a core chemistry-agnostic project with satellite projects targeting short-term objectives and rapid feedback loops. This approach would allow faster learning cycles and enable high-risk, potentially disruptive research to progress without being constrained by traditional funding structures.

4.3.1 Advances needed to meet the challenges

Addressing the challenges outlined above requires a coordinated, multi-dimensional approach that combines scientific, technological and strategic advances across the battery innovation ecosystem. The following priorities are identified to accelerate the development and deployment of new chemistries and cell concepts:

Europe should establish a coordinated framework of practices and resources to ensure that emerging chemistries are developed evaluated in a consistent, transparent and comparable manner. Within such a framework, new systems would be tested under harmonised conditions, employing common cell formats, cycling protocols, and safety procedures, so that results obtained in different laboratories can be meaningfully compared. This level of consistency is currently lacking Performance would be systematically benchmarked against reference systems (such as state-of-the-art LIBs or standard sodium-ion cathodes and anodes) to make the relative strengths and still existing gaps of each chemistry visible. At the same time, advanced characterisation and modelling would be integrated to provide deeper insight into interfacial behaviour, degradation mechanisms, and safety in a coordinated fashion. An essential addition to this framework would be the introduction of structured decision points. After a defined testing phase, each chemistry would be evaluated based on its remaining roadblocks, and strategies to overcome them would be assessed. If critical showstoppers emerge, further development could be discontinued. This will concentrate resources on the most promising directions. Finally, all data generated within this framework should be made FAIR (findable, accessible, interoperable, and reusable), ensuring that knowledge created benefits the entire European R&I community rather than remaining confined to individual projects.

Second, the integration of digital tools and MAPs is essential. By combining multi-scale modelling, HT experiments and artificial intelligence, Europe can significantly shorten the trial-and-error cycles that currently characterize research in post-LIB systems. Importantly, digital workflows should not only optimize for electrochemical performance but also integrate sustainability and manufacturability constraints, ensuring that promising laboratory concepts can realistically progress to industrial deployment.

Third, eco-design principles must be embedded at the earliest stages of research. Safe, Sustainable, and Recyclable by Design approaches should guide material selection, electrolyte formulation and electrode design, anticipating European regulations on hazardous substances, and ensuring recyclability is intrinsic rather than an afterthought. Minimizing the carbon footprint during production and extending the product's useful life must also be considered. To achieve this, it is essential that chemists, materials scientists, recycling experts, and regulatory bodies collaborate closely from the outset of innovation projects. Throughout the development process, applying LCA can help guide sustainable decisions, from raw material sourcing to end-of-life recycling.

A fourth priority is the strengthening of interdisciplinary collaboration. New chemistries cannot be developed in isolation from manufacturing innovations or smart functionalities. For instance, self-healing coatings or embedded sensing could mitigate the instabilities of lithium–sulphur systems, while digital twins could help integrate solid-state electrolytes into scalable production lines. Bringing these different strands together in joint projects will be critical to overcoming bottlenecks that no single discipline can resolve.

Finally, the funding framework must evolve to reflect the high-risk, exploratory nature of new chemistries. Current European projects are often too rigid, with long cycles that slow down iteration and discourage failure. A more agile approach is needed, based on a core chemistry-neutral umbrella programme that provides continuity, complemented by smaller, short-duration satellite projects dedicated to rapid testing of specific hypotheses. This “fail fast and learn” philosophy would allow Europe to test a broader portfolio of ideas while focusing sustained investment on the most promising directions.

4.4 Forward vision

The exploration of new chemistries and technologies is essential to Europe’s long-term energy storage strategy and must be pursued strategically rather than speculatively. To date, no dedicated cluster of projects under this theme exists; instead, various consortia work on early-stage concepts in a decentralized manner, and collaboration between chemistry-focused and technology- or system-level projects remains limited.

There is strong consensus on the need for clearer evaluation frameworks, better coordination, and more agile funding mechanisms. Novelty alone is insufficient justification for research investment. Instead, new chemistries and technologies must be assessed on their added value compared to current LIBs in terms of sustainability, supply chain resilience, safety, application-specific performance, and local (EU) sourcing potential. Traditional labels based solely on active material or electrolyte type, or charge carrier, no longer suffice to meaningfully categorize emerging battery technologies. The hybrid classification proposed in Battery 2030+, based on new shuttle ions and new cell concepts, provides a structured starting point for assessing maturity and technical characteristics.

However, for strategic evaluation and prioritization, additional dimensions must be considered, including for instance material origin (including CRM-free and PFAS-free considerations), target applications (from grid storage and mobility to aerospace), and processing and manufacturability implications. Metrics used to assess new chemistries and technologies should capture both holistic advantages and isolated figures of merit like energy density. Practical challenges such as impurity sensitivity, separator compatibility, water tolerance, and manufacturability must be addressed early in the development cycle, ideally alongside early electrochemical testing, to avoid late-stage failures. Consistent benchmarking is essential, necessitating standardized evaluation frameworks and test protocols to compare performance and trade-offs across diverse chemistries and technologies.

Overall, this requires a shift in funding structures toward more agile and risk-tolerant models that support exploratory research with fast feedback loops—embracing a “fail fast and learn” philosophy rather than prolonged support of underperforming approaches. Finally, regulatory readiness must be built in from the outset, as evolving frameworks—such as PFAS restrictions, REACH regulations, and CRM strategies—will shape the viability of today’s innovations. This aligns with Battery 2030+ vision beyond 2035 to pioneer CRM- and PFAS-free battery chemistries and technologies. The focus must shift from “what is possible” to “what is valuable” scientifically, industrially, and societally across short-, medium-, and long-term horizons.

Collaboration across interdisciplinary research themes ensures that insights from manufacturing and recycling processes effectively inform the discovery and development of novel battery materials and emerging chemistries. Advanced digital tools for predicting the impacts of material choices and manufacturing parameters on final battery performance are progressively reducing reliance on empirical trial-and-error approaches, thereby optimizing production efficiency, scalability, and the overall R&D process.

As the Battery 2030+ initiative advances, functional tools and platforms for accelerated materials discovery developed within the successfully completed BIG-MAP project (2020–2024) are now extended under the FULL MAP project. This extension integrates critical factors such as recycling, critical raw materials (CRMs), and environmental impacts including toxicity directly into the material discovery workflows. This holistic approach is pivotal to delivering scalable and sustainable battery chemistries and technologies that facilitate cost-effective, climate-neutral recycling and reuse of battery components.

The novel materials, next-generation chemistries, and cell concepts envisioned within Battery 2030+ drive the necessity for innovative recycling paradigms. These will encompass reconditioning and reuse of active materials and electrodes, thereby supporting the circular economy objectives central to Horizon Europe's sustainability agenda. This integrated approach directly contributes to Horizon Europe's impact pathways by enhancing the EU's strategic autonomy in CRMs, reducing the carbon footprint of battery manufacturing by at least 30% by 2030, and increasing recycled content in batteries in line with EU regulatory targets. Furthermore, the project aligns with the European Green Deal by promoting climate neutrality, resource efficiency, and sustainable industrial competitiveness within the battery sector.

To pave the way for such a shift, close collaboration among material suppliers, cell and battery manufacturers, and application and recycling stakeholders is essential to accommodate all the above constraints when researching and developing new battery chemistries and technologies. Cross-cutting areas are responsible for ensuring that all R&D&I efforts consider the feasibility of scaling up new materials and battery cell concepts, as well as the potential for recycling and reusing battery components at low cost and through climate-neutral approaches. Looking forward, to enable smart, coordinated development of next-generation chemistries and technologies, the following goals are proposed.

In the short-term (2025–2027), efforts will focus on overcoming fundamental challenges specific to each chemistry; defining a multi-dimensional classification scheme for battery technologies based on cell and battery architecture, material strategy, and application targets; launching early-stage platforms for systematic testing of low-TRL chemistries and technologies under controlled and comparable conditions; beginning de-risking work on manufacturability, safety, and impurity tolerance early in the development pipeline; and identifying "red flags" for early discontinuation of unviable concepts.

In the medium-term (2027–2030), the focus will shift to advancing TRLs with respect to performance, manufacturability, sustainability, scalability, and safety; demonstrating the feasibility of promising chemistries and technologies in larger-format prototypes under real-use conditions such as pouch or cylindrical cells; building cross-disciplinary collaborations that better link battery chemistry and materials science research with manufacturing, functionality, and recycling expertise; aligning new chemistry and technology R&D with regulatory roadmaps, especially for PFAS, CRM, and end-of-life standards; establishing structured technology roadmaps for at least three promising new chemistries and technologies; and evaluating techno-economic and lifecycle impacts.

In the long-term (2030 and beyond), the aim is to deliver novel solutions that unlock markets underserved by LIB technology—such as seasonal stationary storage, long-duration backup, and air mobility; position European research consortia as global leaders in at least one alternative battery chemistry or technology; integrate successful new chemistries and technologies into industrial pilot production lines and digital battery passport systems; contribute to international standards and certification processes for beyond-LIB technologies; and enable industrialization within Europe of new battery chemistries and technologies.

5.MANUFACTURING AND DIGITAL TWINS

Collaboration across interdisciplinary research themes ensures that insights from manufacturing and recycling inform the discovery and development of novel battery materials. Advanced digital tools are increasingly replacing trial-and-error methods by predicting how manufacturing affects battery performance, improving efficiency and scalability[214].

The Battery 2030+ initiative integrates considerations such as recycling, critical raw materials, and toxicity into material discovery workflows. This ensures that newly discovered materials are compatible with both current and emerging battery manufacturing processes. The holistic approach supports the development of scalable and sustainable batteries by enabling cost-effective, climate-neutral manufacturing chains that facilitate efficient recycling and reuse. This integrated approach contributes directly to Horizon Europe’s impact pathways by strengthening the EU's strategic autonomy in critical raw materials, cutting the carbon footprint of battery manufacturing by at least 30% by 2030, and increasing the share of recycled content in batteries in line with EU regulatory targets. The initiative aligns with the European Green Deal by promoting climate neutrality, resource efficiency, and sustainable industrial competitiveness in the battery sector.

5.1 Introduction

The current chapter ensures that all research approaches consider the feasibility of scaling up new materials and battery cells, their manufacturability, and the potential for recycling and reusing battery components at low cost and through climate-neutral approaches. As outlined in the EU Batteries Regulation (Regulation (EU) 2023/1542) 215 , which entered into force on 18 February 2024, sustainable manufacturing is a central element. In response, the Battery 2030+ initiative's Manufacturing and Digital Twins theme links physical battery production with digital models to enhance control, traceability, and integration across the battery life cycle.

A Digital Twin is a model that is continuously updated with real-time data, data-driven system that enables inference of unobservable parameters, such as coating quality from calendar pressure, improving process understanding and optimization. Two Battery 2030+ projects-**BatCAT** and **BATTwin**-are advancing this vision. BatCAT is developing a modular digital twin architecture connecting key battery production stages and incorporating real-time sensor data and semantic data spaces to enable traceability, performance prediction, and predictive quality control. It focuses on both lithium-ion and vanadium redox flow batteries and aligns with EU digital product passport (DPP) requirements, due by 2027, by generating FAIR-compliant data.

BATTwin builds on this by integrating simulation-based models, decision-support systems, and ontology-driven data structures. It emphasizes sensorised pilot lines and is creating a scalable, modular digital twin platform operating at both process and system levels.

Together, these projects aim to deliver efficient, adaptive, and digitally connected manufacturing systems, linked to R&D, DPPs, and recycling. However, challenges remain—many pilot lines lack sensor integration and harmonized workflows.

Manufacturing is the vital bridge between material discovery and deployment. Yet, its role is evolving far beyond traditional production. In the future, manufacturing will increasingly integrate smart functionality—embedding sensors that enable monitoring, optimization, and adaptive performance.

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[214] Pradeep Kumar Dammala, Kamil Burak Dermenci, Anish Raj Kathribail, Poonam Yadav, Joeri Van Mierlo, Maitane Berecibar, A critical review of future aspects of digitalization next generation Li-ion batteries manufacturing process, *Journal of Energy Storage,* **74**, Part B, 109209, ISSN 2352-152X, 10.1016/j.est.2023.109209 (2023).

[215] REGULATION (EU) 2023/1542 OF THE EUROPEAN PARLIAMENT AND OF THE COUNCIL of 12 July 2023 concerning batteries and waste batteries, amending Directive 2008/98/EC and Regulation (EU) 2019/1020 and repealing Directive 2006/66/EC: https://eur-lex.europa.eu/legal-content/EN/TXT/PDF/?uri=CELEX:32023R1542

At the same time, new paradigms such as recycling, remanufacturing, and design-for-disassembly will make manufacturing central to achieving circularity and resource efficiency. Digital twins are a key enabler of this transformation, making this bridge smarter, faster, and more sustainable. As BatCAT and BATTwin evolve, the focus will shift from pilot projects to industrial-scale implementation. Scaling, standardization, and integration across the value chain will be critical. Through this Europe can strengthen its leadership in digitalized, circular battery production.

5.2 Current Status

Manufacturing of battery cells

Given projected European demand of 800 to 1,300 GWh by 2030[216], a production capacity of two TWh would result in significant overcapacity. The market ramp-up of electromobility is progressing more slowly than initially anticipated. At the same time, growing overcapacity in Asia is putting additional pressure on cell prices. Early challenges faced by initial European production projects have dampened investor confidence, leading to the cancellation of many planned initiatives. European battery cell production faces a range of obstacles, including high energy and capital costs, as well as a shortage of manufacturing know-how. Nevertheless, analysis suggests that Europe can position itself as a competitive production hub - supported by policy measures such as the new battery regulation, which mandates CO_2 footprint disclosures and recycling requirements[217]. Despite these hurdles, there remains an urgent need to scale up production to manufacture billions of battery cells within just a few years. This scale-up must be economically viable, environmentally sustainable, and flexible enough to accommodate ongoing advances in cell design and materials chemistry. While the challenge is significant, the goal is achievable - with digital twins serving as key enablers in the process.

This perspective focuses on the manufacturing of battery cells, their components, and materials. Novel manufacturing methods of battery cells[218] are also addressed in this Roadmap from the standpoint of digitalisation, where the integration of digital twins of both the cell and the manufacturing process acts as a key enabler to accelerate and optimize manufacturability of new cell architectures, novel discovered materials as well as integration of advanced sensor functionalities[219].

The manufacturing routes for lithium-ion battery (LIB) cells can be broadly categorised into three stages: electrode production, cell assembly, and cell finishing[220]. Electrodes are typically produced through organic-solvent-based roll-to-roll casting of a slurry onto a metallic current collector, followed by drying and calendaring to achieve the desired thickness[221]. Among these steps, coating and drying are the most cost-intensive[222]. Dryers are generally limited to three chambers to ensure homogeneity, as multiple variations can arise, and the tension of the collectors can also have an effect. The introduction of the three-stage drying profile—based on the influence of film adhesion and compactness at low and high drying rates (LDR and HDR)—has reduced manufacturing defects such as cracks, foil crumbling, and non-uniformity, while improving drying consistency and cost-

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[216] Link, S.*et al.,* Feasibility of meeting future battery demand via domestic cell production in Europe. *Nature Energy*. **10**, pages 526–534, https://www.nature.com/articles/s41560-025-01722-y, (2025).

[217] Wicke, T. *et al.,* Forecasting the ramp-up of battery cell production in Europe: A risk assessment model. *Frauenhofer ISI*, https://www.isi.fraunhofer.de/en/blog/themen/batterie-update/batterie-zell-produktion-europa-hochlauf-risiko-bewertung-gescheiterte-projekte.html (2025).

[218] Ayerbe, E., *et al.,* Digitalization of Battery Manufacturing: Current Status, Challenges, and Opportunities. *Advanced Energy Materials,* 10.1002/aenm.202102696 (2021).

[219] Energy Storage Solution-an Overview | Sciencedirect Topics, https://www.sciencedirect.com/topics/engineering/energy-storage-solution.

[220] Heimes, H.H. *et al. Lithium-ion battery cell production process.* PEM der RWTH Aachen University; DVMA, Aachen, Frankfurt am Main (2018).

[221] Kwade, A. *et al.,* Current status and challenges for automotive battery production technologies. *Nature Energy*. **3** (4), 290–300, 10.1038/s41560-018-0130-3 (2018).

[222] Küpper, D. *et al.,* The Future of Battery Production for Electric Vehicles, https://www.bcg.com/publications/2018/future-battery-production-electric-vehicles.

effectiveness[223,224]. Dry air or nitrogen gas are commonly used for rapid drying, and more recently UV[225] or infrared radiation has been applied for greater efficiency. The solvent N-methyl-2-pyrrolidone (NMP) is typically employed, but it is toxic, flammable, and has a high boiling point (202 °C). This has led to increasing interest in aqueous processing routes within the scientific community, as well as exploration of alternative processing methods[226].

The dry coating technique has garnered significant attention and demonstrated promising prospects for the battery industry as a new path towards sustainability[227,228]. Until now, several other representative methods have been employed to realize solvent-free concepts in battery electrode manufacturing. These methods include pulsed laser[229], sputtering deposition[230,231] and extrusion. Nevertheless, while solvent-free concepts in battery electrode manufacturing show great promise, further studies and research are required before they can be effectively scaled up and applied in industrial settings.

During the cell assembly phase of battery manufacturing, critical steps such as stacking and electrolyte filling take place. These steps are considered time-consuming and economically significant due to their impact on the overall production process. After cell assembly, the cell enters the cell finishing phase, where formation step takes place. This step is held in controlled chambers and is cost-intensive, affected by factors such as variations in material quality, manufacturing parameters, and cell design, but necessary to improve battery performance and lifetime[232].

Slurry mixing/dry mixing technology listed with maturity highest to the left and most experimental to the right				
	Planetary mixer	Twin Screw Extruder	TDS Mixer	Dry Mixer
Adoption	*****	***	**	*
Slurry production method	Batch: Semi continuous with buffer tanks.	Continuous	Batch: Semi continuous with buffer tanks.	Batch
Adaptability	Easy to switch mixed material.	It requires high quality and stability of raw materials.	Easy to change different products but	Easy to change different products but

[223] Jaiser, S. *et al.,* Development of a three-stage drying profile based on characteristic drying stages for lithium-ion battery anodes. *Drying Technology*, *35*(10), 1266–1275. 10.1080/07373937.2016.1248975 (2017).
[224] Jaiser, S. *et al.,* Impact of drying conditions and wet film properties on adhesion and film solidification of lithium-ion battery anodes. *Drying Technology*, **35** (15), 1807–1817. 10.1080/07373937.2016.1276584 (2017).
[225] Pfleging, W. Recent progress in laser texturing of battery materials: a review of tuning electrochemical performances, related material development, and prospects for large-scale manufacturing**,** *International Journal of Extreme Manufacturing***, 3** (1)**,** 10.1088/2631-7990/ABCA84 (2021).
[226] 24M Technologies, Reinventing Lithium-Ion Battery Cell Manufacturing, https://24-m.com/technology/.
[227] El Khakani, S. *et al.,* Melt-processed electrode for lithium-ion battery. *Journal of Power Sources.* **454**, 227884, 10.1016/j.jpowsour.2020.227884 (2020).
[228] Lu, Y. *et al.,* Dry electrode technology, the rising star in solid-state battery industrialization. *Matter.* **5** (3), 876–898, 10.1016/j.matt.2022.01.011 (2022).
[229] Yan, B. *et al.,* Li-rich thin film cathode prepared by pulsed laser deposition. *Scientific Reports.* **3** (1), 3332, 10.1038/srep03332 (2013).
[230] Chiu, K.-F., Lithium cobalt oxide thin films deposited at low temperature by ionized magnetron sputtering. *Thin Solid Films.* **515** (11), 4614–4618, 10.1016/j.tsf.2006.11.073 (2007).
[231] Baggetto, L. *et al.,* Fabrication and characterization of Li–Mn–Ni–O sputtered thin film high voltage cathodes for Li-ion batteries. *Journal of Power Sources.* **211**, 108–118, 10.1016/j.jpowsour.2012.03.076 (2012).
[232] Winter, M., The Solid Electrolyte Interphase – The Most Important and the Least Understood Solid Electrolyte in Rechargeable Li Batteries. *Zeitschrift für Physikalische Chemie.* **223** (10-11), 1395–1406, 10.1524/zpch.2009.6086 (2009).

	Easy to redo production.	Difficult to switch mixed material. Difficult to redo the production.	takes time for pipeline cleaning. Easy to redo production.	takes time for pipeline cleaning. Easy to redo production
Maintenance	Complicated structure and limited maintenance.	Complicated structure, large wear, maintenance cost is high.	Compact system, simple structure, maintenance cost is low.	Medium wear. Medium maintenance.
Energy consumption	Big Power, long time production. Energy consumption is large per mix.	Short slurry production period, low energy consumption.	Short slurry production period, low energy consumption.	Short dry mixing period, low energy consumption per mix.
Investment	Single machine capacity is limited. Huge investment.	The machine is complicated and requires high precision of dosing. Big investment.	The capacity in single machine is big as its dependent on tank size, less investment.	Single machine capacity is limited, medium investment needed.
Space occupation	Highest footprint, and height requirements.	High footprint	Lowest, compact and small	Medium footprint

Slurry mixing/dry mixing technology listed with maturity highest to the left and most experimental to the right				
Viscosity handling	High	Highest	Low to High	N/A
Relative degree of sensorisation	****	*****	*****	***

Coating technologies listed with maturity: highest to the left and most experimental to the right			
	Tandem coater	Simultaneous coater	Dry coater
Throughput	High	High	Low
CAPEX/OPEX	High	Medium (half the number of dryers)	Low (No dryers needed)
Relative degree of sensorisation	******	***	**
Throughput	High	High	Low

Formation Cycler technology listed with maturity: highest to the left and most experimental to the right			
	Conventional Formation Cycler	Regenerative capable Formation Cycler (recovers discharge energy back to grid or uses it for charging other cells)	ML/AI enhanced regenerative Formation Cycler
CAPEX	High	High	Medium
Electricity consumption	High	Medium	Low ((due to shorter formation time)
Time for formation	Long	Long	Short

In addition, to facilitate the connection between advanced materials discovery, battery interface genomes and manufacturability, interfaces must be established across research domains to enable efficient exchange of FAIR[233] data and metadata. The development of infrastructure, along with ontologies, protocols and standards, will be instrumental in this effort.

Eco-design principles, such as designing cells for easy disassembly to facilitate component and material recycling, will be integrated at both the cell design and manufacturing stages. Harmonised protocols and standards will be critical for evaluating and ensuring sustainability of manufacturing processes. Among existing energy storage technologies, LIBs remain the most versatile and widely adopted, offering unmatched energy density across a wide range of applications[234,235,236,237,238]. However, due to the geographically uneven distribution of raw material resources and associated price volatility, the LIBs value chain is under significant pressure. These constraints are fuelling two parallel directions of innovation. On one hand, there is growing interest in alternative battery chemistries that could complement or, in some cases, substitute LIBs for targeted applications. On the other, advanced recycling strategies are gaining momentum, with the goal of recovering high-quality secondary raw materials that can be reintegrated into the manufacturing chain. Together, these efforts are shaping a more resilient, circular, and sustainable energy storage ecosystem.

SIBs have recently gained attention due to the greater abundance and lower cost of sodium compared to lithium[239].

Solid-state batteries (SSBs) are attracting increasing attention as promising next-generation technologies due to potential to enhance safety and energy density, thereby accelerating the adoption of EVs. Similarly, anode-free lithium batteries (AFLBs) are gaining popularity, offering high gravimetric

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[233] Wilkinson, M.D. *et al.,* The FAIR Guiding Principles for scientific data management and stewardship. *Scientific data.* **3**, 160018, 10.1038/sdata.2016.18 (2016).
[234] Steen, M., Lebedeva, N., Di Persio, F., Boon-Brett, L. *EU competitiveness in advanced Li-ion batteries for e-mobility and stationary storage applications - opportunities and actions.* Publications Office of the European Union, Luxembourg (2017).
[235] Energy Storage Solution - an Overview | ScienceDirect Topics, https://www.sciencedirect.com/topics/engineering/energy-storage-solution.
[236] Pillot, C., The Rechargeable Battery Market and Main Trends 2011-2020; presentation (2019).
[237] Duffner, F. *et al.,* Post-lithium-ion battery cell production and its compatibility with lithium-ion cell production infrastructure. *Nature Energy.* **6** (2), 123–134, 10.1038/s41560-020-00748-8 (2021).
[238] Liu, Y., *et al.,* Current and future lithium-ion battery manufacturing. *iScience.* **24** (4), 102332, 10.1016/j.isci.2021.102332 (2021).
[239] Tapia-Ruiz, N. *et al.* ,2021 roadmap for sodium-ion batteries. *Journal of Physics: Energy.* **3** (3), 31503, 10.1088/2515-7655/ac01ef (2021).

energy density, lighter and thinner cells, simplified manufacturing processes and improved sustainability.

In parallel, lithium-sulphur batteries (LSBs) remain a strong focus on research due to their high theoretical specific capacity, low material costs and non-toxicity composition. However, their commercial viability continues to be limited by challenges such as capacity fade and short cycle life. Other battery technologies, including lead acid, redox flow, sodium-sulphur (Na-S)[264] systems remain commercially relevant or are under active development[240].

While LIBs continue to serve as the industry benchmark, it is crucial to acknowledge that current design and manufacturing strategies optimised for LIBs may not be directly transferable to other chemistries. Nevertheless, many underlying manufacturing challenges and guiding principles are shared across these technologies, offering valuable synergies for cross-cutting innovation and scalability.

Cell design

Current battery cell designs primarily follow three main formats: cylindrical, pouch, and prismatic. Among cylindrical cells, the 18650 and 21700 geometries are the most widely adopted, while newer variants such as the 32xxx and 46xxx series incorporate modern advancements, including tabless electrode-to-terminal connections, to enhance performance, thermal management, and manufacturability. Prismatic cells are manufactured in a range of sizes, with recent innovations favouring the blade-type format, particularly suited for EV applications. In the battery energy storage systems (BESS) sector, there is a growing trend toward high-capacity cells (>500 Ah per cell), often featuring custom dimensions designed to optimize container space and thermal management, or to provide tailored solutions that encourage long-term supplier partnerships.

These evolving cell designs aim to improve thermal management, packing efficiency, and high-rate performance, while also reducing manufacturing complexity and costs. Larger-format cells offer notable advantages, including a reduced total cell count, minimized equipment requirements, fewer potential failure points within battery packs, and increased production efficiency. However, they also pose challenges—most notably, a heightened risk of heterogeneous degradation mechanisms that can compromise performance and longevity.

One alternative design approach gaining traction is the Unified Cell concept introduced by PowerCo [PowerCo - Battery-Tech Network]. This strategy is based on a flexible, standardized cell geometry capable of supporting multiple chemistries across various vehicle platforms. By enabling different performance configurations within a unified manufacturing process, the concept delivers cost-effective scalability across a broad range of applications.

To further optimize both cell design and performance, a deeper understanding of the underlying physical and electrochemical processes at both the microscale and macroscale is essential. In this context, digital tools and advanced modelling techniques can play a critical role, providing insights that guide material selection, structural design, and operational strategies across the battery lifecycle.

Integration of Digital Twins and Modelling into cell manufacturing and design

Computational modelling and Artificial Intelligence (AI) will be leveraged to develop digital twins for both novel cell geometries and current or advanced manufacturing routes. This strategy aims to reduce – or potentially eliminate – reliance on traditional trial-and-error methodologies. By creating fully digital representations of products and manufacturing analogues, and seamlessly linking them, it becomes possible to achieve deeper insights into key process parameters and their influence on final cell performance. These virtual counterparts will also support improved control of battery manufacturing facilities and production lines.

[240] Grey, C.P., Hall, D.S., Prospects for lithium-ion batteries and beyond-a 2030 vision. *Nature Communications.* **11** (1), 6279, 10.1038/s41467-020-19991-4 (2020).

Modelling of battery cells and their components has become integral to the design and optimisation process. These models are essential for comprehending cell behaviour, performance characteristics, and identifying areas for enhancement. The advent of digital twins, virtual representation of actual battery cells linked to their physical counterparts, has further revolutionised cell and pack control systems, enabling real-time monitoring and control. Physics-based models are extensively employed to optimize battery electrode and cell performance. Significant efforts have been directed toward methods that refine electrodes microstructure, aiming to understand the impact of nanoscale to mesoscale inhomogeneities on the durability of LIBs[241,242].

Microstructure-resolved, physics-based models are increasingly used to reconstruct electrode microstructures in order to investigate the interplay between structure and electrochemical performance: These models shed light on how heterogeneity influence critical variables such as charge transfer, electrolyte concentration, and local current density. The design of electrode microstructure plays a vital role in determining the performance of the cell, yet the relationship between manufacturing parameters and resulting microstructure remains complex and challenging to simulate.

Key manufacturing steps including mixing, coating, drying and calendaring, are inherently multiphysics (e.g., involving viscous flow, evaporation, precipitation, fracture mechanics) and multiphase (solids, liquids, gasses) in nature. While some progress has been made in physics-based simulation of these processes, pack-sphere models remain the state-of-the-art. However, these models often yield microstructure that differ significantly from the true morphologies observed via microscopy.

For cell design optimisation, the widely adopted pseudo-two-dimensional (p2D) continuum model, pioneered by Newman and colleagues, remains a foundational approach[243,244]. Advances in computational power have enabled extensions of this approach to pseudo-four-dimensional (p4D) meshes [245], allowing researchers and designers to incorporate the effects of cell design features, such as tabs and electrode overhangs, as well as heterogeneous aging phenomena throughout the cell.

Current focus areas include establishing robust connections between model parameters and controllable manufacturing process parameters. A notable development in this direction comes from the UK company Polaron[246,247]. Such linkage is vital for practical optimisation workflows aimed at refining manufacturing processes to achieve desired outcomes.

In parallel, four-dimensional (4D)-resolved finite element method (FEM) models, based on electrode microstructures generated from manufacturing simulations, have been reported. These models capture lithiation/delithiation heterogeneities during battery cycling to manufacturing parameters

[241] Harris, S.J., Lu, P., Effects of Inhomogeneities—Nanoscale to Mesoscale—on the Durability of Li-Ion Batteries. *The Journal of Physical Chemistry C.* **117** (13), 6481–6492, 10.1021/jp311431z (2013).
[242] Meng, J. *et al.,* Advances in Structure and Property Optimizations of Battery Electrode Materials. *Joule.* **1** (3), 522–547, 10.1016/j.joule.2017.08.001 (2017).
[243] Doyle, M., Fuller, T.F., Newman, J., Modeling of Galvanostatic Charge and Discharge of the Lithium/Polymer/Insertion Cell. *Journal of The Electrochemical Society.* **140** (6), 1526–1533, 10.1149/1.2221597 (1993).
[244] Newman, J., Tiedemann, W., Porous-electrode theory with battery applications. *AIChE Journal.* **21** (1), 25–41, 10.1002/aic.690210103 (1975).
[245] Ciria Aylagas, R., *et al.,* cideMOD: An Open-Source Tool for Battery Cell Inhomogeneous Performance Understanding. *Journal of The Electrochemical Society.* **169** (9), 90528, 10.1149/1945-7111/ac91fb (2022).
[246] www.polaron.ai
[247] Kench, Steve *et al.,* Li-ion battery design through microstructural optimization using generative AI. *Matter,* **7** (12) 4260 – 4269, 10.1016/j.matt.2024.08.014 (2024).

such as slurry formulation and degree of calendaring[248, 249, 250]. While these models have not yet integrated into real-time cell operations, they offer strong potential as core components of future digital twin frameworks, delivering valuable insights for cell design optimisation and enhancing battery management.

Challenges in parameter identification for accurate physics-based models have spurred interest in data-driven or ML approaches.[251]These methods develop models directly from observations, capturing complex relationships without explicit physical knowledge. ML techniques are predominantly applied to estimate parameters like SoH, remaining useful life (RUL) and end of life (EOL)[252]. While some exceptions exist, recent research has focused heavily on early prediction of cell lifetime[253], although the high data requirements for model training remain a significant hurdle.

The overarching trend is toward constructing models that balance efficiency and accuracy. Hybrid models, combining physics-based and data-driven techniques, leverage the strengths of both approaches. Physics-Informed Neural Networks (PINNs) integrate physical laws into neural network architectures, allowing incorporation of prior knowledge and governing equations. PINNs have demonstrated promising results in accurately predicting battery performance and safety, offering efficient and accurate modelling solutions. By employing hybrid models and PINNs[254], researchers aim to develop robust models that effectively capture battery cell intricacies, providing accurate predictions for lifetime, performance optimisation, and overall battery management.

Integrating data from sensors, simulations, and other sources, digital twins offer continuous and accurate information about cell performance and state. This real-time monitoring capability enables prompt detection, early issue identification and proactive maintenance strategies. Furthermore, digital twins facilitate control and optimisation of cell operations. By simulating various operating scenarios and applying advanced control algorithms, optimal strategies for maximizing performance, efficiency, and durability can be explored.

Digital twins of battery cells empower manufacturers to closely monitor and manage performance by providing a comprehensive understanding of cell behaviour. They support informed decision-making, predictive maintenance, and the implementation of advanced control strategies.

A digital twin for cell manufacturing is a powerful tool that combines data collection, processing, and integration with advanced models to create a virtual representation of the battery production process and associated machinery. This enables real-time decision-making aimed at improving product quality, production efficiency, and process control.

Moreover, digital twins can also assist in the development and design of production plan. For example, the arrangement of deflection rollers or the mechanical concepts for web control can be optimised at an early stage of planning. During actual operation, the digital twin can serve as a soft sensor**,**

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[248] Liu, C., *et al.,* An experimentally-validated 3D electrochemical model revealing electrode manufacturing parameters' effects on battery performance. *Energy Storage Materials.* **54**, 156–163, 10.1016/j.ensm.2022.10.035 (2023).

[249] Shodiev, A. *et al.* ,4D-resolved physical model for Electrochemical Impedance Spectroscopy of Li(Ni1-x-yMnxCoy)O2-based cathodes in symmetric cells: Consequences in tortuosity calculations. *Journal of Power Sources.* **454**, 227871, 10.1016/j.jpowsour.2020.227871 (2020).

[250] Chouchane, M., Rucci, A., Lombardo, T., Ngandjong, A.C., Franco, A.A., Lithium-ion battery electrodes predicted from manufacturing simulations: Assessing the impact of the carbon-binder spatial location on the electrochemical performance. *Journal of Power Sources.* **444**, 227285, 10.1016/j.jpowsour.2019.227285 (2019).

[251] Xing, W.W. *et al.,* Data-Driven Prediction of Li-Ion Battery Degradation Using Predicted Features. *Processes.* **11** (3), 678, 10.3390/pr11030678 (2023).

[252] Hsu, C.-W., *et al.,* Deep neural network battery life and voltage prediction by using data of one cycle only. *Applied Energy.* **306**, 118134, 10.1016/j.apenergy.2021.118134 (2022).

[253] Rieger, L.H., *et al.,* Understanding the patterns that neural networks learn from chemical spectra, 10.26434/chemrxiv-2023-8pfk5 (2023).

[254] Nicodemus, J., Kneifl, J., Fehr, J., Unger, B., Physics-informed Neural Networks-based Model Predictive Control for Multi-link Manipulators. *IFAC-PapersOnLine.* **55** (20), 331–336, 10.1016/j.ifacol.2022.09.117 (2022).

supplementing physical sensors by providing additional operating data. This offers the dual benefit of reducing the need for physical sensors and accessing measurement data from hard-to-reach areas within the machinery.

The digital twin for battery cell manufacturing typically comprises four core elements:

- Data: Refers to large volumes of real-time information gathered throughout the manufacturing process. This includes data from sensors, equipment, and other relevant sources collected continuously.
- Models: Based on a deep understanding of the underlying physics and operational parameters of the production system, models enable simulation, prediction, and optimisation of critical variables, supporting informed decisions.
- Infrastructure: Includes the necessary hardware (e.g., servers, storage systems) and software platforms and tools for data management, analytics, and visualisation.
- Communication Protocols: Ensure seamless, real-time data exchange between the digital twin and physical equipment or systems.

By integrating these elements, the digital twin provides manufacturers with a powerful tool for optimising production efficiency, quality, and control strategies. It also enables real-time monitoring, analysis, and decision-making, ultimately leading to improved productivity, cost reduction, and enhanced overall performance in battery cell manufacturing[255].

A significant body of work exists on physics-based and ML models addressing the key steps of the lithium-ion battery (LIB) manufacturing process. For instance, analytical models have been developed to estimate the rheological properties of slurries[256]. To understand particle suspensions within slurries, both bi-dimensional Monte Carlo (MC) methods [257,258,259,260] and Brownian Dynamics (BD) approaches [261,262,263] have been proposed. Additionally, 3D-resolved Coarse-Grained Molecular Dynamics models have been used to predict the influence of formulation parameters, solid content, and active material particle size distribution on slurry microstructure[264].

Homogeneous Computational Fluid Dynamics (CFD) models have been employed to simulate the drying process of electrode coatings, specifically to analyse binder migration during solvent evaporation[265]. The Discrete Element Method (DEM) has been applied to study the effect of calendaring parameters on the evolution of electrode microstructure — either by resolving only the

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[255] Ayerbe, E., Berecibar, M., Clark, S., Franco, A.A., Ruhland, J., Digitalization of Battery Manufacturing: Current Status, Challenges, and Opportunities. *Advanced Energy Materials*, 2102696, 10.1002/aenm.202102696 (2021).
[256] Ma, F., *et al.,* Microrheological modeling of lithium-ion battery anode slurry. *Journal of Power Sources.* **438**, 226994, 10.1016/j.jpowsour.2019.226994 (2019).
[257] Valleau, J.P., Card, D.N., Monte Carlo Estimation of the Free Energy by Multistage Sampling. *The Journal of Chemical Physics.* **57** (12), 5457–5462, 10.1063/1.1678245 (1972).
[258] Foulkes, W.M.C., *et al.,* Quantum Monte Carlo simulations of solids. *Reviews of Modern Physics.* **73** (1), 33–83, 10.1103/revmodphys.73.33 (2001).
[259] Yang, B., *et al.,* Equilibrium Monte Carlo simulations of A1–L10 ordering in FePt nanoparticles. *Scripta Materialia.* **53** (4), 417–422, 10.1016/j.scriptamat.2005.04.038 (2005).
[260] Liu, Z., Mukherjee, P.P., Microstructure Evolution in Lithium-Ion Battery Electrode Processing. *Journal of The Electrochemical Society.* **161** (8), E3248-E3258, 10.1149/2.026408jes (2014).
[261] Zhu, M., Park, J., Sastry, A.M., Particle Interaction and Aggregation in Cathode Material of Li-Ion Batteries: A Numerical Study. *Journal of The Electrochemical Society.* **158** (10), A1155, 10.1149/1.3625286 (2011).
[262] Cerbelaud, M. *et al., Numerical* and experimental study of suspensions containing carbon blacks used as conductive additives in composite electrodes for lithium batteries. *Langmuir: the ACS journal of surfaces and colloids.* **30** (10), 2660–2669, 10.1021/la404693s (2014).
[263] Cerbelaud, M., Lestriez, B., Videcoq, A., Ferrando, R., Guyomard, D., Understanding the Structure of Electrodes in Li-Ion Batteries: A Numerical Study. *Journal of The Electrochemical Society.* **162** (8), A1485-A1492, 10.1149/2.0431508jes (2015).
[264] Lombardo, T. *et al., Accelerated* Optimization Methods for Force-Field Parametrization in Battery Electrode Manufacturing Modeling. *Batteries & Supercaps.* **3** (8), 721–730, 10.1002/batt.202000049 (2020).
[265] Lombardo, T., Ngandjong, A.C., Belhcen, A., Franco, A.A., Carbon-Binder Migration: A Three-Dimensional Drying Model for Lithium-ion Battery Electrodes. *Energy Storage Materials.* **43**, 337–347, 10.1016/j.ensm.2021.09.015 (2021).

spatial distribution of active material[266]or by explicitly modelling both active material and carbon-binder domains. Electrolyte infiltration has also been investigated through 3D-resolved Lattice Boltzmann Method (LBM) simulations[267,268,269,270]. In addition, several 3D-resolved process models have been reported, advancing the understanding of physical phenomena during electrode manufacturing[271].

With regard to process optimisation, recent literature has introduced approaches for multi-objective optimisation and inverse manufacturing design[272]. The challenge of the computational cost associated with high-fidelity, physics-based models is increasingly being addressed through machine learning[273]. Data-driven methods can also enhance the interpretability of complex manufacturing processes.[274]

For instance, convolutional neural networks (CNNs) combined with X-ray imaging have been applied for internal wrinkle detection during electrode manufacturing.

Despite these advancements, there remains a lack of integration between machine-level and process-level models in battery manufacturing. Bridging this gap requires the coupling of multiscale models to capture the full manufacturing value chain. Machine models, which simulate the operational behaviour of equipment, must be integrated with process models, which focus on the physical and chemical transformations occurring during production. A promising path forward lies in combining physics-based and data-driven models within a hybrid modelling framework[275]. Physics-based models offer fundamental insights into the underlying physical mechanisms, while ML approaches can extract patterns from large data sets and handle system complexity. The integration of these modelling paradigms will allow the development of robust digital twin platforms, empowering researchers and manufacturers to make more informed, data-driven decisions throughout the battery manufacturing chain.

The production of battery electrodes involves multi-scale, multi-physics processes, each influenced by numerous parameters. While Design of Experiments (DoE) methods are still widely used for optimisation and scale-up, achieving higher control and efficiency requires comprehensive process knowledge, driven by automated data acquisition, robust data infrastructure, and advanced data processing. This includes increased sensorisation to capture relevant data with high speed and accuracy. Parameters such as electrode thickness and density are routinely measured at the macroscopic level, but evaluating electrode microstructure — including pore size, binder distribution, and particle packing — remains challenging, particularly in real-time. The development of real-time

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[266] Sangrós Giménez, C., Schilde, C., Froböse, L., Ivanov, S., Kwade, A., Mechanical, Electrical, and Ionic Behavior of Lithium-Ion Battery Electrodes via Discrete Element Method Simulations. *Energy Technology.* **8** (2), 1900180, 10.1002/ente.201900180 (2020).
[267] Wu, M.-S., Liao, T.-L., Wang, Y.-Y., Wan, C.-C., Assessment of the Wettability of Porous Electrodes for Lithium-Ion Batteries. *Journal of Applied Electrochemistry.* **34** (8), 797–805, 10.1023/B:JACH.0000035599.56679.15 (2004).
[268] Chu, C.-M., Liu, C.-Y., Wang, Y.-Y., Wan, C.-C., Yang, C.-R., On the evaluation of the factors influencing the rate capability of a $LiCoO_2$|Li battery. *Journal of the Taiwan Institute of Chemical Engineers.* **43** (2), 201–206, 10.1016/j.jtice.2011.10.015 (2012).
[269] Bhatnagar, P.L., Gross, E.P., Krook, M., A Model for Collision Processes in Gases. I. Small Amplitude Processes in Charged and Neutral One-Component Systems. *Physical Review.* **94** (3), 511–525, 10.1103/PhysRev.94.511 (1954).
[270] Shodiev, A. *et al., Designing* electrode architectures to facilitate electrolyte infiltration for lithium-ion batteries. *Energy Storage Materials.* **49**, 268–277, 10.1016/j.ensm.2022.03.049 (2022).
[271] Lombardo, T. *et al., The* ARTISTIC Online Calculator: Exploring the Impact of Lithium-Ion Battery Electrode Manufacturing Parameters Interactively Through Your Browser. *Batteries & Supercaps.* **5** (3), 10.1002/batt.202100324 (2022).
[272] Duquesnoy, M. *et al., Machine* learning-assisted multi-objective optimization of battery manufacturing from synthetic data generated by physics-based simulations. *Energy Storage Materials.* **56**, 50–61, 10.1016/j.ensm.2022.12.040 (2023).
[273] Duquesnoy, M. *et al., Functional* data-driven framework for fast forecasting of electrode slurry rheology simulated by molecular dynamics. *npj Computational Materials.* **8** (1), 1–9, 10.1038/s41524-022-00819-2 (2022).
[274] Liu, K. *et al., Feature* Analyses and Modeling of Lithium-Ion Battery Manufacturing Based on Random Forest Classification. *IEEE/ASME Transactions on Mechatronics.* **26** (6), 2944–2955, 10.1109/TMECH.2020.3049046 (2021).
[275] Arcelus, O., Franco, A.A., Perspectives on manufacturing simulations of Li-S battery cathodes. *Journal of Physics: Energy.* **4** (1), 11002, 10.1088/2515-7655/ac4ac3 (2022).

microstructural characterisation tools is still ongoing and often constrained by high costs and technical limitations.

A key objective is to establish a correlation between macro-scale sensor data and micro-scale electrode properties, which remains an open challenge. Progress in sensor technologies, data infrastructure, and analytical methods for microstructural evaluation will be essential to achieving this goal. Advancements in these areas will enable more precise control and optimisation of electrode manufacturing processes, ultimately resulting in improved cell performance, production efficiency, and product quality[276].

Finally, given the interconnected nature of battery manufacturing facilities, where various physical assets interact dynamically, it is essential to establish clear communication protocols and standardised interfaces. These standards enable seamless interaction and data exchange between physical systems and their corresponding digital twins, improving interoperability across platforms and ensuring that diverse components can work together effectively.

5.3 Challenges

Developing next-generation battery cell designs that minimize waste, energy use, and emissions is critical for achieving sustainable, low-carbon manufacturing. In this context, multiphysics modelling plays a vital role across the entire battery design and production process. However, to fully realize its potential, advanced computational platforms are needed, integrating multi-scale physicochemical models with AI to simulate and optimize lithium-ion battery (LIB) manufacturing, from cell design to production.

Emerging functionalities, such as self-healing materials and embedded sensors, as well as new materials discovered through projects like BIG-MAP (2021-2024), can be explored through computational science. Yet, integrating these innovations requires a rethinking of current manufacturing processes.

Innovative technologies, such as metallic lithium anodes, thin-film electrodes, and solid electrolytes, show promise but demand fundamental changes in how batteries are manufactured. This calls for a holistic approach that considers design, performance, sustainability, and scalability.

The Battery 2030+ initiative promotes such forward-thinking, recognising the need to “think outside the box” to prepare for future, as-yet-undefined battery technologies. Although we can’t predict exact future manufacturing concepts, we can identify key enabling tools and methods that will shape them.

This Roadmap identifies several major challenges in battery production:

- Enhancing current manufacturing methods (e.g., roll-to-roll processes) by improving efficiency, reliability, and scalability.
- Developing novel manufacturing techniques to support next-generation chemistries and materials not yet fully commercialised.
- Scaling up from lab to pilot and industrial production, an area where digital twins and modelling tools can dramatically reduce time and resource demands.
- Overcoming these challenges requires close collaboration between academia, industry, and policymakers. Only by uniting these efforts can we enable efficient, scalable, and sustainable battery manufacturing chains, which lies at the heart of the Battery 2030+ vision.

Based on the preceding analysis, the following challenges can be outlined:

Current LiB manufacturing relies heavily on trial-and-error methods, which significantly increase development time, cost, and material waste. The industry is characterized by high capital investments

[276] Zanotto, F.M. *et al., Data* Specifications for Battery Manufacturing Digitalization: Current Status, Challenges, and Opportunities. *Batteries & Supercaps.* **5** (9), e202200224, 10.1002/batt.202200224 (2022).

and economies of scale, leading to large, inflexible gigafactories specialized in a limited range of chemistries and cell formats. This specialization results in difficulties adapting to new chemistries, mainly due to high start-up costs and elevated scrap rates. Additionally, there is limited support for small-scale production, which hinders the introduction of novel materials and emerging technologies into the market. To address these challenges, urgent needs include reducing solvent and energy consumption, minimizing material scrap, accelerating time-intensive processes—particularly formation—and enabling recyclable cell designs that facilitate the reuse of components.

Looking ahead, next-generation battery chemistries and architectures will require more flexible and rapid manufacturing methods. This shift involves transitioning from traditional wet-chemical routes to solid-state processes, alongside HT production and rapid prototyping capabilities. However, integrating self-healing materials and embedded sensors introduces new challenges related to scalability, automation, cost efficiency, and recyclability. Manufacturing must also preserve functional microstructures within complex three-dimensional and mesoscale composite materials. Achieving these goals will necessitate a transition towards predictive manufacturing tools and low-carbon processes, with particular emphasis on direct recycling and design-for-reuse of structural cell components.

Scaling up manufacturing from laboratory settings to gigafactories remains constrained by a limited understanding of the relationships governing scale. A lack of standardization further complicates scale-up efforts and hampers system interoperability. Moreover, the current focus on large-scale production often neglects the need for flexible, modular systems that support smaller-scale or distributed manufacturing. As manufacturing scales up, the complexity of testing increases, demanding enhanced quality control measures. Key enablers to support improved scale-up include the adoption of digital tools such as digital twins, which can simulate and predict relationships between process parameters and battery performance. Alongside these, advanced modelling and simulation techniques help reduce reliance on costly physical prototyping and iterative trials.

Despite their promise, implementing digital twins in battery manufacturing faces significant barriers. Accurately parameterizing models requires substantial time and investment, though these challenges can be mitigated through simulation-based optimization and the application of machine learning on large datasets. A further limitation is the lack of integration between machine-level models (focusing on equipment behaviour) and process-level models (addressing material transformations), reducing the overall effectiveness of digital twin approaches. While physics-based models offer high fidelity, they are often computationally expensive and require extensive domain expertise. Current research is focusing on hybrid modelling approaches—such as physics-informed machine learning—model simplification techniques and leveraging high-performance computing resources. Meanwhile, inline sensing technologies mostly capture macro-scale properties like coating thickness; however, real-time, non-destructive characterization of microstructural features remains an unmet need in manufacturing.

Standards and protocols

Developing standards and protocols for process development and monitoring is crucial for achieving efficient and sustainable battery manufacturing. While commercial considerations may sometimes hinder standardization, the benefits—such as improved interoperability, reproducibility, reduced scrap, and enhanced sustainability and profitability—strongly support its adoption.

The long-term goal is to enable automated data collection using standardized, interoperable formats for integration into the Battery 2030+ Electronic Lab Notebook (ELN)[277], based on BattINFO[278,279] as developed within former BIG-MAP project and extended to battery manufacturing.

[277] BIG-MAP, electronic lab notebook, big-map-notebook.eu.
[278] Clark, S., Bleken, F.L., Friis, J., Anderson, C.W., Battery INterFace Ontology (BattINFO), BIG-MAP (2021).
[279] BIG-MAP, BattINFO ontology, https://github.com/BIG-MAP/BattINFO.

Key challenges for data alignment and integration in the Digital Product Passport include integrating heterogeneous data across different formats and stakeholders, ensuring real-time sensor data integration into digital twins despite inconsistent sensing infrastructures, and standardizing metadata schemas and ontologies across diverse production environments and chemistries.

5.3.1 Advances needed to meet the challenges

To meet the demands of efficiency, sustainability, and adaptability, battery cell manufacturing must undergo rapid and coordinated transformation.

In the short term, priority must be given to developing green, low-CO_2 production routes that are compatible with large-scale industrial deployment and fully integrated with recycling strategies. At the same time, manufacturing systems must remain flexible enough to accommodate emerging chemistries such as Na-ion and solid-state batteries. Cost-effective, scalable processes—such as dry electrode coating—need to be implemented with demonstrated reproducibility, accompanied by reliable data on long-term performance.

Process innovation will require the adoption of fast, bidirectional screening tools to accelerate optimization, while strengthening supply chains for manufacturing equipment to ensure robust and uninterrupted production capacity. Equally important is the creation of open-source, interoperable software that can handle standardized data, models, and machine interfaces in full alignment with *Battery Passport* requirements. Advanced digital tools, including AI-enhanced modelling approaches such as Reduced-Order Models (ROMs) and Physics-Informed Neural Networks (PINNs), will be essential for guiding design and process optimization, supported by automated parameterization pipelines.

Smart manufacturing will be further enabled by real-time sensing. Deploying intelligent sensors across the value chain will generate microstructural and process data that improve monitoring, quality assurance, and resource efficiency.

The benefits for Europe’s battery industry will be far-reaching: higher sustainability and production efficiency, improved material optimization through rapid structure–property screening, faster transitions from laboratory to gigafactory scale, enhanced cell quality with predictable lifetimes, and greater resilience to evolving battery technologies. Together, these advances will position Europe at the forefront of digitalized, sustainable, and circular battery manufacturing.

5.4 Forward Vision

The future of battery manufacturing lies in developing next-generation cell designs that minimize waste, energy consumption, and emissions—driving the transition toward sustainable, low-carbon production. Achieving this requires a paradigm shift from incremental optimization to predictive, data-driven, and fully integrated design and manufacturing.

In the short-term (2025-2027): The focus will be on building the foundations for digital twin workflows and data interoperability. This will involve implementing DoE/DoS methods selectively within specific modelling and characterization activities to improve reproducibility and reduce trial-and-error. Initial semantic metadata structures for equipment, process steps, and key variables will be developed, aligned with existing ontologies or simple controlled vocabularies. Version-controlled data pipelines will be set up to ensure traceability from experiments and simulations to digital twin models. Small-scale pilots will be run to test the integration of sensor data with digital twin components, focusing on feasibility rather than full-scale AI control. Common gaps and requirements for scaling up digital twins across use cases, such as cell assembly and slurry preparation, will be documented.

In the medium-term (2027-2030): The work will progressively expand digital twin coverage across connected manufacturing stages, for example from slurry preparation to early cell assembly, with a focus on selected process segments where data availability and infrastructure readiness allow meaningful integration. Modular simulation workflows and reusable digital twin components will be developed and aligned, starting with shared parameters and formats for specific cell formats, enabling comparison and benchmarking rather than enforcing full standardization. Proof-of-concept trials will be initiated for adaptive control strategies, using feedback from functional testing and early End-of-Life (EoL) indicators in small-scale or laboratory environments, to assess the feasibility and added value of self-adjusting manufacturing settings.

In the long-term (2030 and beyond): The focus will be on operationalizing interoperable, modular digital manufacturing systems. This will include enabling cross-platform deployment of digital twins by adhering to modular architecture and agreed interface specifications. Semi-automated quality control routines will be deployed using combined sensor data, simulation outputs, and AI models for feedback. Traceable data chains from raw materials through manufacturing and testing will be demonstrated to enable regulatory reporting and Digital Product Passport integration. The work will contribute to the formalization of EU-wide standards for battery manufacturing data, in coordination with emerging regulatory frameworks and industry platforms. Finally, R&D–manufacturing–recycling data exchange pilots will be supported through federated platforms that respect data sovereignty.

Meeting the challenges outlined in this Roadmap requires a holistic transformation of battery cell manufacturing. The current reliance on capital-intensive gigafactories and trial-and-error development hinders adaptability, wastes resources, and slows innovation. To overcome these limitations, Europe must accelerate the adoption of green, low-CO_2 manufacturing routes, integrate recycling and design-for-disassembly at every stage, and embrace flexible production lines that accommodate multiple chemistries and formats.

Digitalization will be the decisive enabler. Tools such as digital twins, hybrid modelling approaches, AI-driven optimization, and interoperable open-source platforms will shorten scale-up timelines, reduce scrap, and increase transparency across the value chain. Smart sensing technologies will provide real-time insights into microstructural evolution, enhancing both quality control and resource efficiency. Together, these advances will pave the way for predictive manufacturing processes that minimize energy and material use while maximizing cell performance and lifetime.

Collaboration across academia, industry, and policymakers will be crucial to align standards, ensure interoperability, and enable a truly circular value chain. The benefits for Europe will be profound: faster transitions from lab-scale prototypes to gigafactory-scale production, improved resilience against raw material constraints, higher manufacturing efficiency, and leadership in the global race for sustainable, digital battery technologies.

6. RECYCLING AND RAW MATERIALS

Interdisciplinary collaboration and advanced digital tools are enhancing battery material discovery by integrating manufacturing and recycling insights. Projects like BIG-MAP have embedded factors such as recycling, critical raw materials (CRMs), and toxicity into workflows. As LIB waste continues to grow and current second-life strategies remain limited, improving recovery and recycling is essential for a resilient, sustainable, and circular battery value-chain.

Cathode optimization remains a key priority due to its disproportionately high manufacturing cost. The Battery 2030+ initiative promotes innovative recycling methods to support circular economy goals and reduce material dependency. As gigafactories begin to generate significant volumes of production scrap, the material is expected to dominate the input stream for recycling, shifting the focus from end-of-life batteries to manufacturing scraps. Addressing this shift will require coordinated efforts in material design, process efficiency, and scalable recycling technologies.

Battery 2030+ treats raw materials and recycling as strategic elements for sustainability. Direct recycling is a major focus due to its efficiency in preserving battery component integrity. Projects like **RENOVATE, REUSE, REVITALISE, STREAMS, CICERO, INERRANT,** and **Li4Life** address various aspects of recycling, from sorting and purification to sustainable material recovery. Additional Horizon Europe and BEPA projects (e.g., REINFORCE, BATTEREVERSE, REBELION, etc.) explore second-life applications and novel recycling technologies.

Projects such as SOURCE, LICORNE, REBORN, and GR4FITE3 align with key EU priorities including phasing out PFAS (e.g., PVDF in LIBs), reducing dependency on CRM imports, and implementing battery passports for digital traceability. Despite progress in KPIs, LCAs, and digital tools, industrial scaling remains a major hurdle. A robust recycling strategy must prioritize production scrap, expected to make up 60% of recyclable input in the EU[280] by the end of this decade, due to the rapid gigafactory expansion. As battery chemistries diversify (e.g., LFP, sodium-ion, solid-state), recycling must adapt to varied material recovery challenges. Often overlooked components like binders, foils, and electrolytes—especially those containing PFAS—require attention under tightening regulations.

Manual disassembly is not scalable; automated sorting and shredding within digitally enabled environments are essential. Mobile, container-based recycling units offer flexible and cost-efficient local solutions. Safety standards for handling cells and end-of-line scrap must be rigorously applied, and recovered materials must meet reintegration quality standards, validated at pilot scale. Digital tools like battery passports and digital twins will be vital for tracking materials, certifying recycled content, and enabling circularity. This makes recycling a design, supply chain, and digital infrastructure challenge. End-of-life batteries must be seen not as waste, but as an important resource to limit the dependencies on primary raw material imports.

Battery 2030+ responds with innovation and systems-level thinking. As gigafactory waste grows and new chemistries emerge, the Roadmap prioritizes scalable recycling, smart reintegration, and transparent metrics. Direct recycling shows significant potential but is still largely carried out on the lab scale, remains challenging for end-of-life batteries, and requires industrial scaling. Hydrometallurgical processes, though more mature, require innovation and broader adoption and can be considered as a bottleneck for a battery circular economy. Future recycling must be flexible to handle various battery chemistries, demanding versatile "omnivore" systems. Apart from critical raw materials from the cathode, graphite recovery should also be prioritized to strengthen Europe's battery sovereignty and global sustainability leadership.

[280] https://www.strategyand.pwc.com/de/en/industries/automotive/recycling-european-battery.html

6.1 Introduction

The development of battery dismantling and recycling technologies with high efficiencies going well beyond the EU Battery Directive 2006/66/EC target of 70%[281] (repealed by the Batteries Regulation (Regulation (EU) 2023/1542[282])) for most battery technologies is essential to ensure the long-term sustainability of the battery economy by 2030. This calls for new, innovative, simple, and low-cost processes targeting a very high recycling rate, low carbon footprint and other environmental impacts, economic viability as well as for logistics and business incentives. In addition, it is an important step towards seeing end-of-life batteries as a resource rather than waste.

To pave the way for such a shift, there will be a direct coupling to material suppliers, cell and battery manufacturers, main application actors, and recyclers to integrate the constraints of recycling into new battery designs and manufacturing processes. These include: (1) design for sustainability (including eco-design, SSbD as well as economic and social aspects considering the whole lifecycle), (2) design-for-dismantling and (3) design-for-recycling approaches. For the inclusion of design strategies, it is important that industrial participation will be brought on board early. In such a way, the Battery 2030+ Roadmap will promote a sustainable and circular economy.

In addition to the current challenges such as battery collection, automated sorting, and dismantling, it is expected in the future that recycling streams will increasingly consist of mixed and cross-contaminated battery chemistries, if the source of the battery waste stream is unknown to the recycler. The currently available hydro-pyro processes can generally only treat specific chemistry. Thus, as one option, further innovation is required to develop “omnivore” hydro-pyro technologies capable of processing variable streams, until labelling clearly identifies the battery chemistry. Hydrometallurgical processes in particular will require further technological advances as well as a greater industry willingness to adapt to novel approaches. There should also be significant focus on the recovery and reuse of graphite (due to its high criticality), similar to critical metals.

Implementation of the design for circularity[283], which incorporates design for sustainability and, more specifically, design for recycling, is to be integrated in the algorithms for automated materials discovery (the input parameters can be the criticality of the raw materials, raw material toxicity, reduced number of elements, and other socioeconomic aspects)[284]. At the same time, both recycling topic and the overarching theme of sustainability need to be accompanied by developing standards and protocols for assessing the economic and environmental validity of recycling processes. This can include also the development of ways to certify carbon footprint and overall sustainability of the complete battery life cycle[285].

6.2 Current Status

The battery recycling industry has developed significantly in the EU since the implementation of the Batteries Directive (Directive 2006/66/EC 286), and, more recently, the Batteries Regulation (Regulation (EU) 2023/1542287). The new regulation, adopted on 12 July 2023 and applicable from 18

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[281] E. Commission, Regulation concerning batteries and waste batteries (2020), https://eur-lex.europa.eu/resource.html?uri=cellar:4b5d88a6-3ad8-11eb-b27b-01aa75ed71a1.0001.02/DOC_1&format=PDF.
[282]Batteries Regulation (Regulation (EU) 2023/1542: https://eur-lex.europa.eu/legal-content/EN/TXT/PDF/?uri=CELEX:32023R1542
[283] Wolf, A. *et al.,* Circular battery design: investing in sustainability and profitability. *Energy Environ. Sci.*, **17**, 8529-8544, 10.1039/D4EE03418J (2024)
[284] Weil, M.; *et al.,* Batteries Europe Task Force Sustainability: Position paper. 2024. Batteries Europe, https://batterieseurope.eu/wp-content/uploads/2024/05/Task-Force-Sustainability.pdf
[285] European Technology and Innovation Platform, Sustainability Position Paper (2021).
[286] Commission Regulation concerning batteries and waste batteries (2020), https://eur-lex.europa.eu/resource.html?uri=cellar:4b5d88a6-3ad8-11eb-b27b-01aa75ed71a1.0001.02/DOC_1&format=PDF.
[287]Batteries Regulation (Regulation (EU) 2023/1542: https://eur-lex.europa.eu/legal-content/EN/TXT/PDF/?uri=CELEX:32023R1542

February 2024, repeals Directive 2006/66/EC and amends Directive 2008/98/EC and Regulation (EU) 2019/1020. It introduces a harmonised framework across all EU Member States and strengthens Extended Producer Responsibility (EPR), making battery producers—or third parties acting on their behalf—financially and operationally responsible for the collection, treatment, and recycling of waste batteries.

As part of the European Commission's "Circular Economy Action Plan", the regulation supports the transition to a more sustainable and resource-efficient battery value chain. It introduces updated battery categories and sets minimum targets for recycled content in new batteries, which will come into effect over the coming years (See Figure 12). To ensure consistent implementation, Commission Delegated regulation (EU) 2025/606[288], entered into force on July 4, 2025, establishes the methodology for calculating and verifying recycling efficiency and material recovery rates, along with the required documentation format.

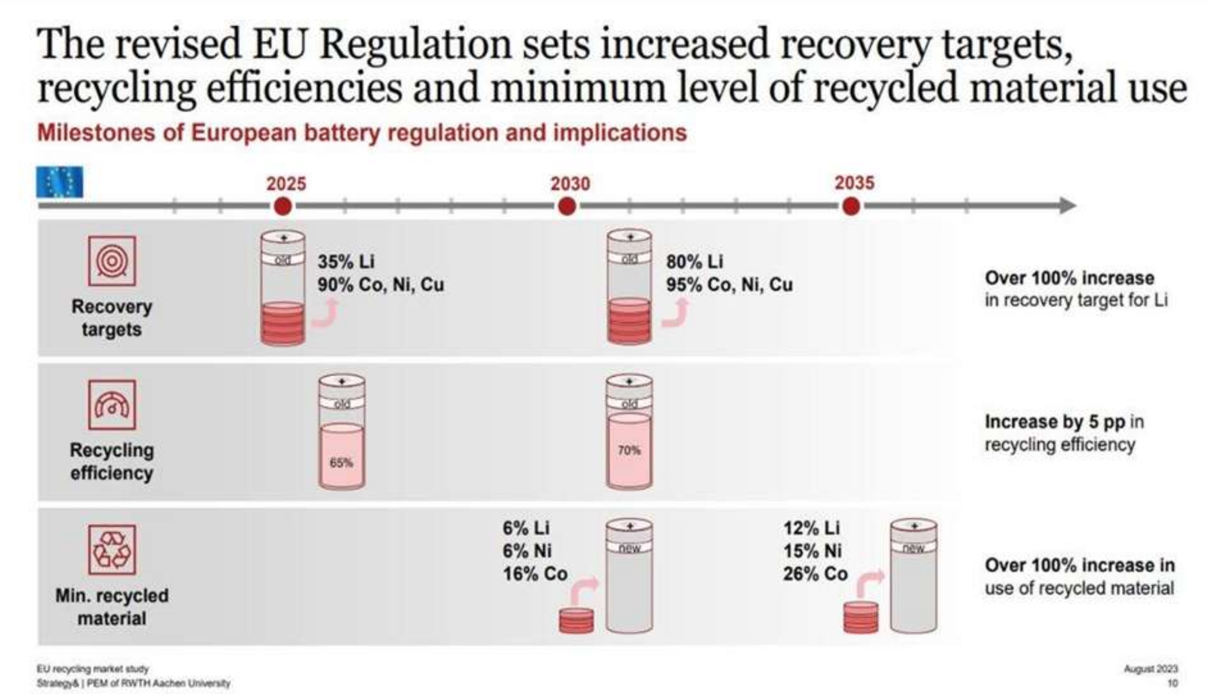

FIGURE 12. Recovery targets, recycling efficiencies and material reuse.

After potential dismantling and sorting into categories according to battery chemistries, the batteries or battery parts are directly fed into the recycling process or further fragmented by physical means (e.g., shredding or grinding). In terms of recycling schemes, depending on the battery chemistry and process chosen, several steps involving physical, mechanical, and/or chemical transformations may be needed. Although each recycler may use variations or combinations of different individual steps, recycling processes (or schemes) are currently classified as shown in Figure 13.

[288] Commission Delegated Regulation (EU) 2025/606: https://eur-lex.europa.eu/legal-content/EN/TXT/PDF/?uri=OJ:L_202500606

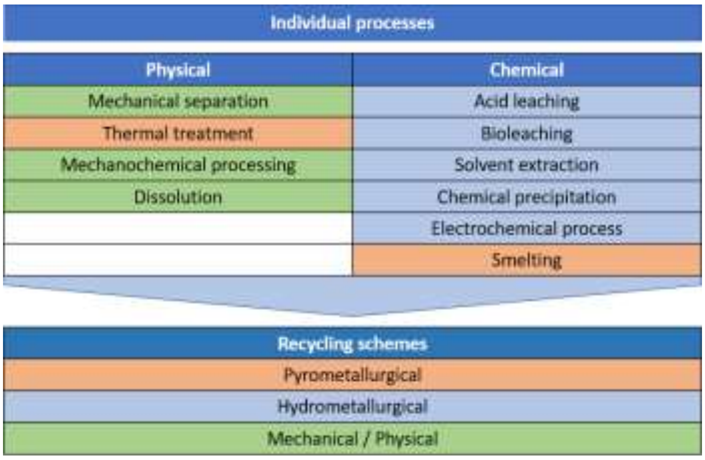

FIGURE 13. Traditional recycling processes and schemes.

6.3 Challenges

Battery collection targets differ by battery type: targets for portable batteries have historically lagged behind automotive ones. Data from the European Environment Agency[289] show collection rates for portable batteries reached only 46–47% by 2022, falling short of upcoming targets under EU regulation (63% by 2027, 73% by 2030). Complex battery product structure increases recycling cost, where current technologies struggle to efficiently separate micro-components and embedded electronics, significantly raising costs and complexity.

The usage of PFAS-based binders is common in current Li-ion batteries. Recycling processes must ensure that PFAS do not enter the environment through different pathways[290,291], and that the binder can be effectively recovered and recycled. Efficient sorting of mixed battery types requires high-throughput, automated detection systems. Future battery design partly addresses this via labelling mandates in the revised Battery Directive.

Inactive components are often neglected, where recovery of inactive cell parts (e.g., separators, electrolytes) remains challenging although necessary to meet recovery targets.
Safe EV battery designs make disassembly complex and costly, reliant on manual labour (which introduces not only scalability issues but also significant safety risks)[292]. Manual disassembly can expose workers to hazardous materials and the risk of electrocution, making automation a key opportunity for improving both efficiency and safety in recycling processes. One particularly risky step is the discharge of EV battery packs, which, if not properly controlled, can lead to overheating, fire, or explosion. Data-driven methods for automated discharge control, such as temperature monitoring and predictive algorithms, could greatly reduce these risks, especially in large-scale operations.

Furthermore, battery passports containing life history data could help predict pack behaviour during discharge, enabling safer and more efficient recycling workflows. Direct recycling remains largely lab-based, and demonstrating its economic benefits poses significant challenges. This novel approach recovers high-value anode and cathode active powders and other components directly from spent cells, separates and reconditions them into battery-grade materials.

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[289] https://www.eea.europa.eu/en/european-zero-pollution-dashboards/indicators/collection-rate-for-portable-batteries-and-accumulators-indicator?utm_source=chatgpt.com
[290] Savvidou, E. K. *et al.,* PFAS-Free Energy Storage: Investigating Alternatives for Lithium-Ion Batteries. Environmental Science & Technology, **58** (50), 21908–21917. 10.1021/acs.est.4c06083 (2024).
[291] Salces, A.M. et al., Evaluation of a Bio-Based Solvent Pretreatment for Sustainable Froth Flotation of Black Mass from Spent Lithium-Ion Batteries. ACS Sustainable Resource Management, 2 (6), 10.1021/acssusresmgt.5c00058 (2025).
[292] https://environment.ec.europa.eu/topics/waste-and-recycling_en

Low-value chemistry batteries, such as LFP and Na-ion, have begun penetrating both stationary and mobile markets. Therefore, the development of highly efficient, low-cost recycling technologies is essential to ensure economically viable and sustainable recycling solutions[293,294].

Methodological challenges remain in prospectively analysing and estimating the economic, ecological, and social impacts of emerging battery technologies.

Specific short/medium-term challenges:

- New battery technologies are expected to enter medium-term markets, including solid-state, lithium-sulphur, redox flow, and metal-air batteries for mobility and stationary applications. Recycling processes will need to adapt to these diverse chemistries and their associated BMS, presenting new challenges; for example, the presence of lithium metal raises safety concerns, potentially requiring process redesigns such as inert gas atmospheres depending on the battery type[295].
- The large-scale transition to aqueous electrode processing is inevitable due to economic and ecological benefits for battery manufacturing, recycling, and active material recovery[296,297,298]. However, obsolete binders and additives must be removed before further recovery steps[299,300].
- Despite recent advances in direct recovery of electrode active materials, additional upgrading of electrode chemistries will often be necessary, as decommissioned batteries typically contain outdated chemistries[301,302].
- Some recycling processes may introduce impurities, such as aluminium or copper fragments from current collectors, into recovered electrodes[303]. While some impurities can occasionally be beneficial[304] impurity avoidance or removal strategies are generally required to produce reusable and competitive electrodes.
- The growing volume of EV batteries on the market has led to emerging business models, including reuse of sorted battery modules or cells to extend service life or enable second-life applications.
- Battery information will increase through advanced BMS, sensor data, and future battery passports. Processes to manage and standardize this data for reuse and recycling are needed.

[293] Peters, J.F., Baumann, M., Binder, J.R., Weil, M., On the environmental competitiveness of sodium-ion batteries under a full life cycle perspective – a cell-chemistry specific modelling approach. *Sustainable Energy & Fuels.* **5** (24), 6414–6429, 10.1039/D1SE01292D (2021).
[294] Peters, J., Baumann, M., Weil, M., Passerini, S., On the Environmental Competitiveness of Sodium-Ion Batteries – Current State of the Art in Life Cycle Assessment. In Titirici, M.-M., Adelhelm, P., Hu, Y.S. (eds.) *Sodium-ion batteries. Materials, characterization, and technology.* Wiley-VCH. Weinheim (2023), pp. 551–571.
[295] Azhari, L., Bong, S., Ma, X., Wang, Y., Recycling for All Solid-State Lithium-Ion Batteries. *Matter.* **3** (6), 1845–1861, 10.1016/j.matt.2020.10.027 (2020).
[296] Li, J. *et al., Water*-Based Electrode Manufacturing and Direct Recycling of Lithium-Ion Battery Electrodes-A Green and Sustainable Manufacturing System. *iScience.* **23** (5), 101081, 10.1016/j.isci.2020.101081 (2020).
[297] Whittingham, M.S., Beyond the Nobel recognition - To a cleaner sustainable future. *Journal of Power Sources.* **473**, 228574, 10.1016/j.jpowsour.2020.228574 (2020).
[298] Vanderbruggen, A. *et al., Automated* mineralogy as a novel approach for the compositional and textural characterization of spent lithium-ion batteries, 10.31223/x53p54 (2021).
[299] Ross, B.J. *et al., Mitigating* the Impact of Thermal Binder Removal for Direct Li-Ion Battery Recycling. *ACS Sustainable Chemistry & Engineering.* **8** (33), 12511–12515, 10.1021/acssuschemeng.0c03424 (2020).
[300] Bai, Y., Muralidharan, N., Li, J., Essehli, R., Belharouak, I., Sustainable Direct Recycling of Lithium-Ion Batteries via Solvent Recovery of Electrode Materials. *ChemSusChem.* **13** (21), 5664–5670, 10.1002/cssc.202001479 (2020).
[301] Xu, P. *et al., Efficient* Direct Recycling of Lithium-Ion Battery Cathodes by Targeted Healing. *Joule.* **4** (12), 2609–2626, 10.1016/j.joule.2020.10.008 (2020).
[302] Xu, P. *et al., Design* and Optimization of the Direct Recycling of Spent Li-Ion Battery Cathode Materials. *ACS Sustainable Chemistry & Engineering.* **9** (12), 4543–4553, 10.1021/acssuschemeng.0c09017 (2021).
[303] Zhang, R. *et al., Systematic* Study of Al Impurity for NCM622 Cathode Materials. *ACS Sustainable Chemistry & Engineering.* **8** (26), 9875–9884, 10.1021/acssuschemeng.0c02965 (2020).
[304] Zhang, R. *et al., Understanding* fundamental effects of Cu impurity in different forms for recovered LiNi0.6Co0.2Mn0.2O2 cathode materials. *Nano Energy.* **78**, 105214, 10.1016/j.nanoen.2020.105214 (2020).

Such information will be valuable for second-life applications and for selectively exchanging aged cells within battery packs.

- The vast quantities of battery systems and modules to be recycled will demand substantial logistical efforts, with transportation significantly increasing costs, safety risks, and CO2 emissions. To address this, decentralized collection and recycling units must be developed, prioritizing lower environmental impact and costs, along with potentially gaining higher societal acceptance. Additionally, a legislative framework must be established to foster and safeguard sustainable design practices, including design for recycling.

Tentative long-term challenges (2030 and beyond):

- Novel battery technologies—such as magnesium-, potassium-, aluminium-, and sodium-based systems—may enter the market. Rapid battery chemistry evolution can render some batteries obsolete, reducing their recycling value and raising challenges for managing these unwanted materials. Conversely, emerging chemistries may increase material criticality (regarding production capacities) due to immature raw material supply chains and limited refinement capacities. Furthermore, recycling processes developed for lithium-based cells will need to be redesigned for chemistries based on other metal ions
- Large volumes of spent batteries will require transforming recycling plants to highly automated processes, covering sorting, dismantling, and the subsequent recycling stages. Generation 4.0 recycling plants will need significant investment and innovation to develop flexible, economically viable processes capable of treating multiple battery sources with different chemistries.
- Recycling technologies must be able to recover advanced intelligent battery components, such as sensors, self-healing materials, and other information-linked parts. New circular economy business ecosystems for reconditioning and reusing recycled products and materials will need to be developed, ideally located near recycling units and decentralized when possible.

6.3.1 Advances needed to meet the challenges

Battery 2030+ aims to transition to a new recycling model centred on comprehensive data collection and analysis, automated pack disassembly down to the cell level, and exploring reuse and repurposing opportunities wherever possible. It also focuses on automated cell disassembly to maximize component recovery, alongside developing selective powder-recovery technologies that recondition powders into battery-grade active materials reusable for automotive and stationary applications, all while significantly reducing logistical efforts.

The "Eco-design preparatory study for batteries"[305], completed in May 2025, provides the European Commission with technical, environmental, and economic analyses of batteries, aligned with relevant European Directives, especially the Eco-design Directive (2009/125/EC)[306]. While environmental sustainability is addressed, social aspects are often insufficiently considered.

Battery 2030+ expands this scope by including social aspects alongside technical, environmental, and economic considerations to ensure comprehensive sustainability, in addition to a technology-neutral approach to accommodate all innovative developments. The initiative also aims to establish a foundation for holistic, sustainable battery design that prioritizes circularity, starting from raw and advanced materials through design for manufacturing and material recycling. The focus extends beyond the use phase to encompass the entire life cycle, applying prospective life cycle assessment (P-LCA) methods and contributing to the definition of rules and standards for the recycling stage.

[305] European Commission, Ecodesign preparatory Study for Batteries, www.ecodesignbatteries.eu
[306] EUR-Lex, Directive 2009/125/EC of the European Parliament and of the Council of 21 October 2009 establishing a framework for the setting of ecodesign requirements for energy-related products Text with EEA relevance (2009), https://eur-lex.europa.eu/legal-content/DE/ALL/?uri=celex%3A32009L0125

Implementing standards and protocols for recyclability is a key element in achieving a circular economy, enhancing recycling efficiency, and reducing dependency on imports. A crucial aspect is the connection between manufacturability and comprehensive battery history information, which directly facilitates the choice of recycling process.

The ambition of Battery 2030+ is to develop a ground-breaking recycling process that advances beyond the current state-of-the-art. Present recycling flows, which rely on pyro- and hydrometallurgical methods involving multiple processing steps, are summarized in Figure 14. Given the increasing diversity of battery designs and chemistries, as well as varying technological readiness levels, a multilateral approach combining pyro-, hydro-, and direct recycling methods is expected to dominate battery recycling over the next decade[307]. However, from a sustainability perspective, there will inevitably be an increased focus on direct recycling techniques, which aim to recover not only the most valuable materials but all components. Moreover, the reliance of hydro- and, in particular, pyrometallurgical processes on market values of metals like cobalt and nickel introduces economic volatility and reduces planning reliability[308]. Recycling of design-to-cost chemistries is not likely to be economically viable via pyro- and hydrometallurgical processes[309].

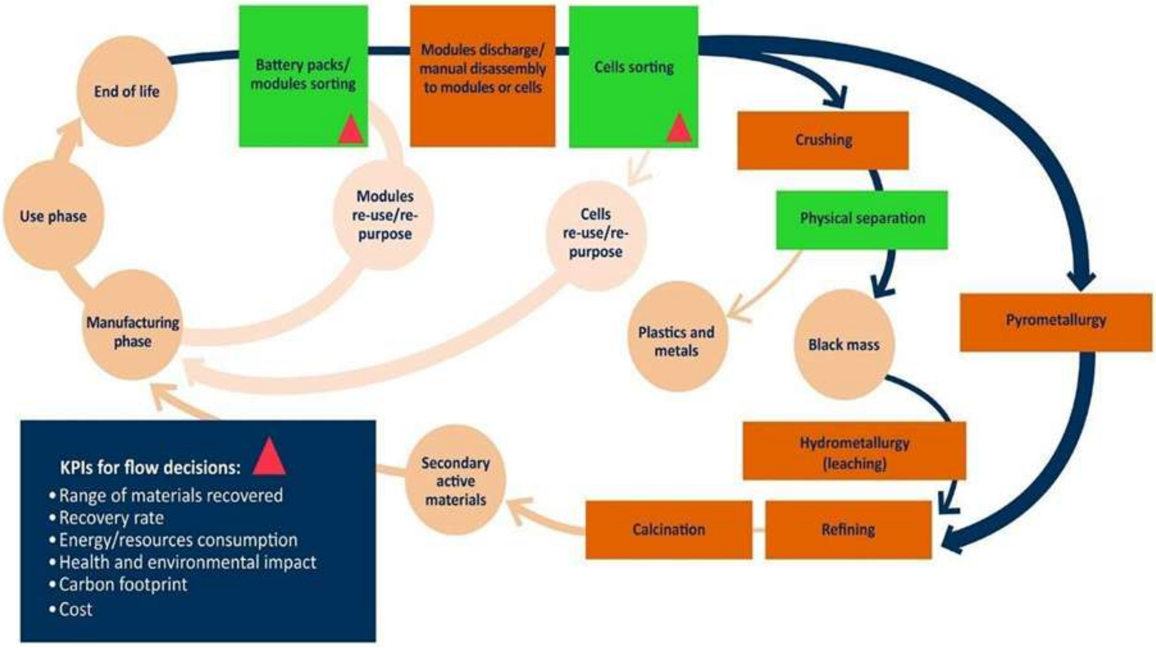

FIGURE 14. Schematics of present recycling processes.

Based on a novel, integrated approach to recycling designed materials, developed in the BIG-MAP project (2020–2024) and further advanced by FULL MAP as of February 2025, as well as on sensor technologies (as described in Chapter 3.1.1. *Sensing*), Battery 2030+ will propose a new model (see Figure 15) founded on the following pillars:

- Data collection and analysis, including information from labels, BMS, sensors, and the battery passport.
- Modern, low-carbon-footprint logistics concepts, including decentralized processing.
- Automated pack disassembly to the cell level.
- Reuse and repurposing wherever feasible.
- Automated cell disassembly to maximize the recovery and purity of individual components.

[307] Harper, G. *et al., Recycling* lithium-ion batteries from electric vehicles. *Nature.* **575** (7781), 75–86, 10.1038/s41586-019-1682-5 (2019).
[308] Thielmann, A. *et al., Batterien* für Elektroautos: Faktencheck und Handlungsbedarf (2020).
[309] Wolf, A. *et al.,* Circular battery design: investing in sustainability and profitability. *Energy Environ. Sci.*, **17**, 8529-8544, 10.1039/D4EE03418J (2024).

- Development of selective technologies for powder recovery, upgrading, and reconditioning into battery-grade active materials, reusable in automotive and stationary applications. Where direct reuse is not possible, precursor synthesis is envisioned, with necessary composition adjustments.
- Future recycling processes, where direct recycling is fully integrated with reuse and binder recycling, enabling a more efficient and sustainable materials loop.
- Integration of design-for-recycling strategies during cell production to support the new recycling model. This implies that design for recycling and design for circularity principles are embedded early in the battery design process.
- Optimised pyrometallurgical and hydrometallurgical processes applied to ultimate waste, aimed at demonstrating the high recovery rates expected for CRMs.
- Stimulated and structured international collaboration.

Direct recycling does not mean a single recycling process, but instead describes a recycling process where the output is the active material rather than a precursor[310]. There will most likely not be a single "one size fits all" direct recycling process but solution tailored to a specific cell chemistry. To properly and consistently assess each process step in terms of economic and environmental impacts—and to ensure the validity of such assessments—a comprehensive framework of standards and protocols will be developed. This will be undertaken in close coordination with other European and international consortia, initiatives, and regulatory bodies.

The overall objective is to establish a harmonised framework for assessing and certifying the economic, environmental, and societal impacts of large-scale battery production, use, and recycling—particularly in high-volume applications such as traction batteries[311].

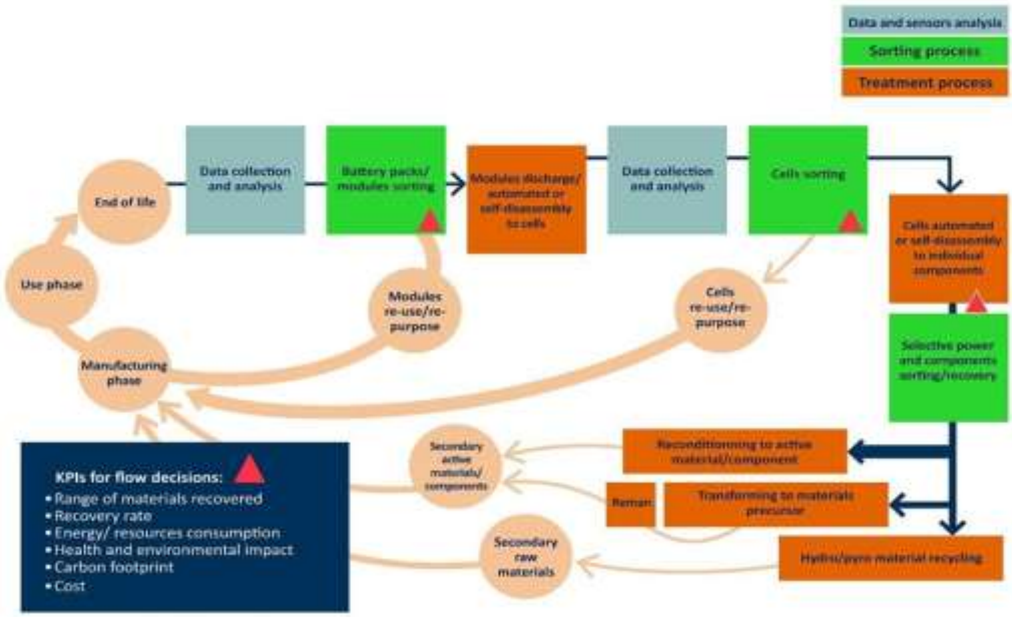

FIGURE 15. Future recycling processes: direct recycling is fully integrated with reuse and binder recycling. While it summarizes the total approach of the complete circularity loop, obviously, not all the steps are currently at the same TRL level.

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310 Hayagan N., et al., Challenges and Perspectives for Direct Recycling of Electrode Scraps and End-of-Life Lithium-ion Batteries, *Chemistry Europe*, 10.1002/batt.202400120 (2024).
311 European Technology and Innovation Platform, Sustainability Position Paper (2021).

Table 1. Current TRL levels and priorities set by Battery 2030+

	TRL	Battery 2030+ priority
Design for sustainability/recycling	3	3
Packs/cells data collection and analysis	2	2
Battery packs/modules sorting	3	2
Fast SoH determination (<30 min)	1	2
Automated disassembly packs/modules	2	2
Re-use/re-purposing/second life echnologies	8	5
Cells sorting	2	2
Cells opening/automated disassembly	2	2
Selective separation/recovery materials from cells	1	1
Reconditioning technologies materials/DR	1	1
Validation materials in automotive/ESS new cells	1	1
Back-up pyro/hydro process if DR not successful	9	6
Recommendations for design/standardisation	3	4
Social approval	3	4

Activities focus on fundamental low-TRL research to implement direct recycling through[312]: Selective material separation and recovery from cells using methods such as cell cutting, shredding, ultrasonic treatment, and froth flotation to recover cathode, anode, electrolyte, and binder materials. Material reconditioning technologies, including tailored processes for cell disassembly, electrode detachment, binder extraction, purification, relithiation, and upgrading/upcycling. Validation of reconditioned materials in new automotive and energy storage system (ESS) cells. Key considerations include process scale-up and integration, definition of relevant KPIs, emphasis on cost-effective battery chemistries (e.g., LFP), and incorporation of Na-ion and solid-state battery chemistries.

6.4 Forward vision

The new recycling process will serve as the foundation for a series of research and innovation (R&I) actions, with the primary objective of implementing direct recycling and design for circularity strategies in the long term (see Figure 16).

[312] Gaolei Wei, *et al.,* Direct recycling of spent Li-ion batteries: Challenges and opportunities toward practical applications, *iScience*, **26**(9), 10.1016/j.isci.2023.107676 (2023).

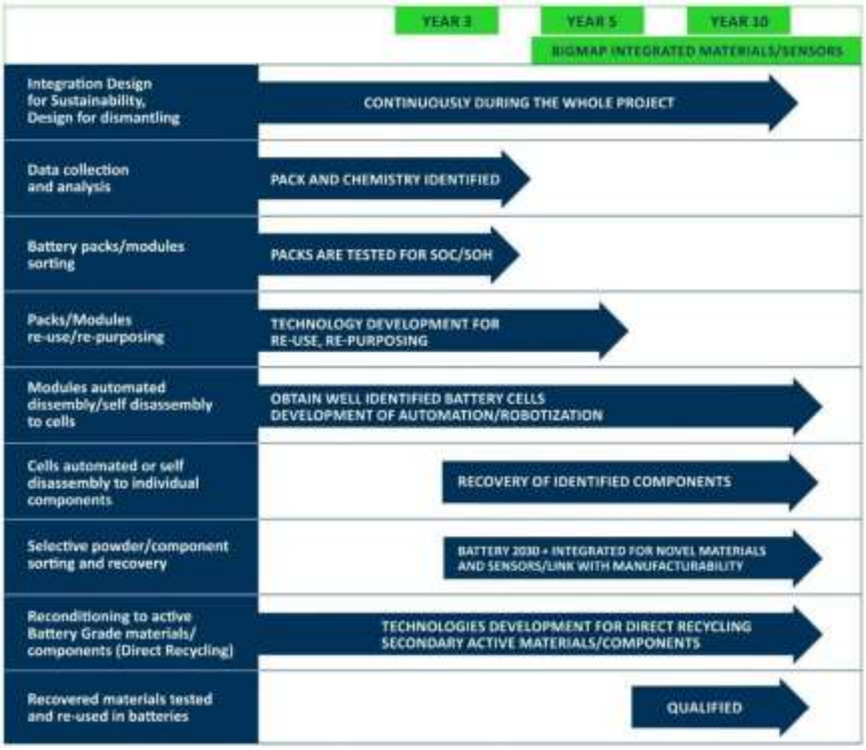

Figure 16. The Ten-Year Roadmap for Recyclability within Battery 2030+

In the short-term (2025–2027): the priority must be on developing scalable solutions that address current and emerging recycling needs, while significantly improving safety through automation, to minimise human exposure to hazardous processes. The majority of recyclable material will originate from production scrap generated during the rapid scaling of gigafactories. Recycling processes must therefore be optimized for these waste streams, with an emphasis on direct recycling technologies and advanced pre-treatment methods, including the recovery of L(M)FP, graphite, and Gen 3b anode materials.

If certain materials or components are not suitable for reconditioning to battery-grade quality—due to structural degradation, impurity levels, or other purity constraints—a fallback alternative in the final stage of the new recycling process could involve their conversion into precursors. These precursors may be modified through adjustments in composition ratios, anticipating future battery chemistries and the requirements of next-generation materials[313].

Parallel development of technologies for binder removal, fluorine recovery, and material purification will be crucial to meeting both regulatory and performance requirements. Hydrometallurgy-based processes capable of treating varying battery volumes and different chemistries, including the recovery and valorisation of graphite, must also be developed and scaled. These processes should be flexible and modular to accommodate the evolving composition of battery waste in the early years of recycling market development.

Initial integration of recycling flows into manufacturing lines should begin. To consistently assess environmental and economic impacts, harmonized KPIs, as well as LCA and LCC (Life Cycle Costing) frameworks, must be established early. These will form the basis for long-term tracking of circularity and impact and will help identify potential goal conflicts.

In the medium-term (2027–2030): By 2027, the reintegration of recycled materials into pilot and pre-industrial manufacturing must become standard practice, with quality and consistency validated under

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[313] Fichtner, M. *et al., Rechargeable* Batteries of the Future-The State of the Art from a BATTERY 2030+ Perspective. *Advanced Energy Materials*, 10.1002/aenm.202102904 (2021).

realistic production conditions. Recycling routes will need to adapt to emerging chemistries, such as sodium-ion and solid-state systems, each of which presents unique separation and recovery challenges.

Hydrometallurgical processes must continue to evolve to handle increasing and diversified battery waste streams, ensuring high recovery rates across a range of materials and chemistries. Special emphasis should be placed on graphite recovery and its valorisation, enabling its reuse or repurposing into new applications, thereby closing another critical materials loop. Pilot and pre-industrial recycling plants will play a central role in supporting industrial-scale recycling and adapting to changing feedstocks.

To support interoperability and scalability, harmonized recycling standards and digital data structures must be implemented across chemistry families. Battery passports will play a key role by enabling traceability of material origin and recyclability indicators. Importantly, recycling data must feed back into materials discovery and battery design, helping to close the loop between product development and end-of-life strategies.

In the long-term (2030 and beyond): Europe must establish fully circular battery value chains that rely as little as possible on minimal virgin material input. Achieving this will require design-for-recycling principles to be embedded at the cell, module, and system levels from the outset. Material choices must proactively respond to regulatory developments, such as the PFAS phase-out and CRMs strategies, through substitution and recovery innovations.

In parallel, second life applications will play a vital role in extending battery utility and reducing environmental impact, particularly for low-value chemistries that may not justify intensive recycling efforts. These batteries, while less suited for high-performance mobility, can be repurposed for stationary storage, grid balancing, or backup systems, where performance demands are lower but longevity and cost-effectiveness are key. Designing batteries with second-life potential in mind, including concepts from modularity to health diagnostics, will be essential to unlocking this value.

Hydrometallurgical processes still need to be adapted to manage the growing battery volumes expected by 2030, including through innovation strategies that address non-metal components to fully close the material cycles loops.

Digital technologies will be central to enabling both circularity and second-life strategies. AI, ML, and digital twin technologies will optimise battery lifecycles by integrating design, usage, and recycling data into intelligent decision-support systems. Circularity metrics must be embedded into certification schemes and public procurement policies, ensuring that sustainability is incentivized and scaled across the market.

7. DATA AND STANDARDS AS TOOLS FOR COLLABORATION AND INNOVATION

7.1 Introduction

The digital transformation of battery research represents one of the most significant paradigms shifts in materials science and energy storage technology. In the context of Battery 2030+, data serves not merely as a byproduct of research activities, but as a fundamental asset that drives innovation, accelerates discovery, and enables unprecedented collaboration across disciplines, institutions, and sectors.

The complexity of modern battery systems generates vast amounts of heterogeneous data across multiple scales, timeframes, and research domains. This data encompasses experimental measurements, computational simulations, manufacturing parameters, performance metrics, sustainability assessments, and more. The challenge lies not only in the volume and variety of this data, but in transforming it into actionable knowledge that can drive the development of next-generation battery technologies.

Battery 2030+ establishes common frameworks for data management, and sharing. The initiative aims to create a digital ecosystem, where information flows seamlessly between research areas, enabling synergistic discoveries that would be impossible within isolated domains.

The strategic importance of data standardization extends beyond immediate research outcomes. It establishes the foundation for artificial intelligence and machine learning applications, enables reproducible science, facilitates regulatory compliance, and creates pathways for industrial translation. Moreover, it positions European battery research within the global data economy, ensuring competitiveness while maintaining scientific openness and collaboration.

7.2 Current Status

The battery research ecosystem currently produces data at an unprecedented scale and diversity. This data is generated mostly through a combination of electrochemical testing at individual labs and organizations, model-based simulation data, and large-scale research infrastructure such as synchrotron facilities.

On the experimental side, cycling data, impedance spectroscopy, and performance metrics are routinely collected in electrochemical testing facilities. These measurements are complemented by advanced characterization techniques such as x-ray diffraction, Raman spectroscopy, tomography, and high-resolution electron microscopy, which provide detailed insights into the structural, chemical, and morphological evolution of materials during operation. Parallel to this, manufacturing processes are becoming digitally monitored, with real-time sensor data and inline imaging contributing to quality assurance and process optimization. However, the absence of clear standards for linking cycling or state of health to data from these diverse sources presents a significant challenge. Establishing frameworks for data integration and interpretation is essential to fully leverage these complementary approaches. Importantly, field testing and operational monitoring of deployed systems are generating large volumes of real-world usage data, linking laboratory findings to practical performance and degradation profiles.

Comparable progress has been achieved in the computational domain, where diverse modelling approaches generate rich datasets that complement experimental measurements. Atomistic simulations provide parameter sets describing fundamental material properties such as diffusion coefficients, reaction barriers, and electronic structures. At mesoscale and continuum levels, simulations produce detailed descriptions of electrochemical performance under varying conditions.

Machine learning and artificial intelligence extend this landscape further, creating surrogate models that distil complex simulations into accessible forms while also generating synthetic datasets to fill gaps where experiments are limited. The growing field of digital twins builds on this foundation by combining multiphysics simulations with operational data streams, producing continuously updated performance predictions and degradation trajectories. Such computational outputs are increasingly valuable not only for guiding materials discovery and cell design but also for enabling predictive maintenance, optimization of manufacturing processes, and assessment of sustainability across the battery lifecycle.

Equally important is the growing stream of data generated in industrial environments, particularly from BMS deployed in EVs, stationary storage units, and other large-scale applications. These systems continuously record data including voltage, current, and temperature across thousands of operating cycles under highly diverse real-world conditions. When aggregated, BMS data provides insights into usage patterns, degradation modes, and safety-relevant events at scale. Beyond operational monitoring, such datasets can be mined to refine lifetime prediction models, optimize charging strategies, and identify early indicators of failure. Industrial datasets thus form a crucial bridge between controlled research environments and actual field performance.

Considerations of confidentiality and openness remain central to the evolving data landscape. Much of the data generated within industrial contexts is necessarily treated as confidential, reflecting competitive considerations and intellectual property concerns. However, datasets produced within publicly funded research projects represent a different case. To maximize scientific and societal impact, these should be made openly available under permissive licenses that allow broad reuse, analysis, and integration into shared platforms. Ensuring that publicly funded results are openly accessible not only reinforces the principles of transparency and reproducibility but also provides the foundation for the collaborative ecosystem envisioned by Battery 2030+.

Existing Standards and Frameworks

Battery 2030+ has made significant strides in creating common standards and frameworks for structuring, annotating, and exchanging information. A central achievement is the development of the BattINFO ontology[314], which provides a machine-readable representation of battery science. BattINFO formalizes the core concepts, relationships, and properties that span the battery domain, covering electrochemical processes, materials, components, testing protocols, and performance metrics. By offering a consistent semantic backbone, it enables automated reasoning and supports interoperability across datasets, tools, and research domains.

Battery 2030+ standards and frameworks are not being developed in isolation. They are a central part of the global battery community, and alignment with international initiatives is a cornerstone of the strategy. The Battery Parameter eXchange (BPX)[315] format, developed by the UK-based Faraday Institution, provides a widely used standard for exchanging battery model parameters in a structured and transparent way, and its adoption across the modelling community demonstrates how standardized formats can accelerate model calibration, comparison, and re-use. A particularly worthwhile goal is the integration of structural characterization data (e.g., XRD, spectroscopy) with electrochemical (EC) time series, enabling a more holistic understanding of battery behaviour under realistic operating conditions. This could be achieved by adapting a hierarchical data format, such as HDF5, which is well-suited for storing large, complex datasets with multiple interrelated dimensions. HDF5 allows for efficient organization of time-resolved data, metadata, and multi-modal measurements, making it an ideal candidate for harmonizing experimental outputs across techniques. Similarly, the Battery Data Format (BDF)[316], coordinated by Linux Foundation Energy, is establishing a global, community-driven framework for structuring experimental battery test data. By harmonizing

[314] https://github.com/emmo-repo/domain-battery
[315] https://bpxstandard.com/
[316] https://github.com/battery-data-alliance/battery-data-format

with both BPX and BDF, Battery 2030+ ensures that European datasets are directly compatible with the most prominent international efforts, enabling cross-initiative integration and supporting a broader global battery data ecosystem.

These domain-specific initiatives are complemented by more general frameworks that provide robust foundations for FAIR data management. RO-Crate[317], for example, offers a lightweight packaging method for sharing datasets together with rich metadata in a structured, machine-actionable way, improving portability and accessibility across platforms. The concept of FAIR Digital Objects is also highly relevant, offering a unifying mechanism to ensure that battery data can be uniquely identified, linked, and reused across scientific domains.

In addition to research-focused standards, alignment with regulatory frameworks is essential. The EU Battery regulation[318], which requires all industrial batteries placed on the European market to carry a digital passport containing key information about materials, performance, and sustainability, represents a transformative step in linking research data to industrial practice and regulatory compliance. Initiatives such as Battery Pass Data Mode[319] are already piloting methodologies, standards, and governance models for implementing the Battery Passport, with a strong emphasis on interoperability, traceability, and data sovereignty. By engaging with these developments, Battery 2030+ ensures that its data standards not only advance scientific discovery but also contribute directly to meeting upcoming regulatory requirements and supporting the competitiveness of European industry.

Existing Infrastructure and Tools

The practical realization of standards depends on infrastructures and tools that support the collection, management, publication, and integration of battery data. Across the Battery 2030+ community, a layered ecosystem of such resources is emerging, moving from laboratory instruments to open scientific knowledge bases.

At the level of data collection, EMPA has developed a modular software ecosystem that enables standardized acquisition and transformation of battery cycling data across different test systems[320]. The *aurora* suite provides dedicated interfaces for widely used cycler brands, including *aurora-neware* and *aurora-biologic*, which allow users to start, stop, and monitor experiments directly from Python or command-line tools. The *aurora-unicycler* package extends this functionality further by offering a "universal" cycling format: protocols can be defined in Python or JSON and then converted automatically into standardized outputs, including BattINFO-compatible JSON-LD. By lowering the technical barriers to unifying outputs from heterogeneous cyclers, the aurora toolchain supports the FAIR-compliant integration of experimental data into higher-level databases.

IFE has developed CellPy[321] (the open-source python library for reading, homogenizing and processing battery data from different battery cyclers) in a joint effort between industry and researchers. Recent developments include BattINFO-compatibility, speed improvements, and efforts to lower the friction for open-source contributions through outreach, collaboration and code refactoring. The CellPy library is built with the philosophy that it should play well within the Python data ecosystem (for example within data pipelines and orchestrations tools such as Prefect) as well as being an easy and intuitive tool to use for individual battery researchers (for example within a Jupyter or Marimo notebook).

Beyond the laboratory, more general-purpose research data management systems are being adapted for battery science. Kadi4Mat[322], originally designed as a data management platform for materials

317 https://www.researchobject.org/ro-crate/
318 https://eur-lex.europa.eu/eli/reg/2023/1542/oj
319 https://github.com/batterypass/BatteryPassDataModel
320 https://github.com/EmpaEconversion
321 https://github.com/jepegit/cellpy
322 https://kadi.iam.kit.edu/

research, has been refined to support battery-specific use cases. It provides flexible structures for managing both experimental and computational datasets and can be deployed as an internal institutional instance for private use or as a shared public resource. Its modular architecture allows it to integrate smoothly with laboratory workflows while maintaining FAIR-compliant metadata standards.

For long-term archiving and open dissemination, Zenodo[323] has become a central publication platform. Closely connected with Kadi4Mat, it allows researchers to publish curated datasets with persistent digital object identifiers (DOIs), version control, and licensing options. This ensures that results from publicly funded research projects are preserved and openly available under conditions that enable reuse and citation.

At the highest level of integration, the Battery Knowledge Base (BKB)[324] collates data from multiple sources, including Zenodo communities, and enriches it through a semantic media wiki interface. This provides both structured and user-friendly access to a growing body of battery knowledge, enabling researchers to search, compare, and expand information across experimental, computational, and industrial domains. By linking datasets with ontologies such as BattINFO, the BKB transforms distributed resources into a coherent and navigable knowledge graph.

This layered infrastructure forms a continuum from laboratory data collection through institutional management, open publication, and global knowledge integration. It demonstrates how technical standards, when embedded into practical tools, can be translated into a functioning digital ecosystem for battery research.

TABLE 2. Overview of existing battery data standards and infrastructure

Stage	Resource	Scope	Role
Collection	Aurora suite	Interfaces with heterogeneous cyclers (Neware, Biologic, etc.), parses raw data, and provides universal cycling formats	Harmonizes data acquisition at source, ensures raw test data is consistent and machine-readable
Collection	Galv	Specialized platform for collecting and managing cycling data, including metadata and derived parameters	Curates experimental data, supports diagnostics, modelling, and reuse across projects
Harmonization	BattINFO	Formal ontology for battery concepts, relationships, and properties	Provides semantic backbone for interoperability, annotation, and reasoning
Harmonization	BDF	Global framework for structuring experimental battery test data	Enables community-driven standardization and international data exchange
Harmonization	BPX	Parameter exchange format for battery models	Facilitates calibration, validation, and reuse of model parameters
Harmonization	Battery Passport	Regulatory framework and data model for lifecycle traceability of industrial batteries	Links scientific data with regulatory compliance, sustainability, and industrial competitiveness

[323] https://zenodo.org/communities/battery-knowledge-base
[324] https://battery.knowledge-graph.eu/wiki/Main_Page

Management	Kadi4mat	Research data management platform tailored to materials and battery science	Provides FAIR-compliant metadata structures and flexible deployment (internal or public)
Publication	Zenodo	Open repository offering DOI assignment, versioning, and licensing options	Preserves datasets, ensures open access, and enables citation and reuse
Integration	Battery Knowledge Base	Knowledge base combining semantic wiki with linked datasets and ontology alignment	Collates and enriches distributed data, enabling semantic navigation and knowledge graph integration

7.3 Challenges

Although considerable progress has been made in building the foundations of a digital ecosystem for battery research, significant challenges remain before the vision of seamless data integration and reuse can be fully realized. These challenges span technical, organizational, and infrastructural dimensions, reflecting the inherent complexity of both the scientific domain and the research environment in which it operates.

Technical Challenges

One of the most pressing difficulties is the persistence of heterogeneity and fragmentation across the data landscape. Despite efforts to harmonize practices, data formats, measurement protocols, and reporting standards still vary widely across projects and institutions. This lack of uniformity creates barriers to integration and slows down the creation of comprehensive datasets that could enable meta-analysis and cross-project insights. The problem is compounded by the multi-scale nature of battery systems. Connecting atomistic simulations with electrode- or cell-level performance and structural data requires models and computational frameworks capable of bridging scales in a consistent manner. While such approaches are under active development, they are not yet sufficiently mature to support routine cross-scale integration.

Ensuring data quality and consistency poses another challenge. Even small differences in calibration procedures, environmental conditions, or operator practices can introduce systematic errors that compromise the comparability of results across laboratories. Establishing robust quality control and benchmarking procedures is therefore essential but remains resource-intensive. A further difficulty lies in the integration of legacy data. Large volumes of valuable historical measurements exist in formats that are poorly documented, proprietary, or otherwise incompatible with emerging standards. Converting these datasets into FAIR-compliant formats requires significant manual effort and domain expertise, raising questions of feasibility and prioritization.

Organizational Challenges

Beyond the technical domain, there are substantial organizational hurdles to overcome. The culture of academic research often rewards rapid publication over thorough data documentation, sharing, and curation. As a result, many researchers perceive standardization activities as secondary to their core scientific outputs, despite their long-term value to the community. Changing this culture requires a shift in incentives, including recognition of data contributions as legitimate scientific achievements.

Resource limitations exacerbate the problem. Comprehensive data management systems demand investment in infrastructure, skilled personnel, and continuous training. Not all research groups, particularly smaller laboratories, have access to the expertise or funding required to participate fully in standardization efforts. Industrial partners face an additional layer of complexity. While they recognize the benefits of interoperability and open science, they must also protect intellectual property and competitive advantage. Designing data sharing frameworks that balance openness with confidentiality remains a delicate and unresolved issue.

7.3.1 Advances needed to meet the challenges

Overcoming the barriers identified in the previous section requires coordinated advances in technical capabilities, infrastructure development, community practices, and governance. These advances will ensure that the Battery 2030+ community can fully realize the potential of digitalization and establish a sustainable, interoperable, and FAIR-compliant data ecosystem for European battery research.

Technical Advances

A central technical priority is to make it fast and easy for researchers to manage and publish their data in a FAIR-compliant way. Although metadata standards, ontologies, and supporting Python packages already exist, there is still a significant knowledge barrier. Most researchers lack the time or data science expertise required to work with these tools effectively. To overcome this, the technology stack must continue to evolve so that FAIR-compliant practices are embedded seamlessly into laboratory and computational workflows. Instead of requiring researchers to learn new systems, the tools must operate implicitly, capturing metadata, annotating datasets, and preparing files for publication as part of routine experimental or modelling activities.

Progress in automated data annotation and quality control is particularly important. Artificial intelligence and workflow integration can drastically reduce the need for manual intervention, ensuring that datasets are automatically enriched with provenance, checked against community standards, and prepared for publication in repositories without additional overhead. Similarly, lightweight interfaces like electronic lab notebooks, web dashboards, and plug-ins for commonly used equipment or software will play a vital role in lowering the entry barrier and making FAIR data management intuitive.

Equally critical are platforms that streamline the flow of data from collection to dissemination. Computational architectures must support the integration of experimental results, simulations, and field data in a way that requires little to no manual harmonization. These systems should incorporate uncertainty quantification and automated reporting so that results are not only comparable but also trustworthy. Real-time analytics and digital twins offer an additional opportunity, enabling immediate feedback to researchers during experiments and facilitating adaptive designs that improve efficiency and insight.

Ultimately, the goal is to bring data directly to the researchers who need it, without requiring them to become data managers or programmers. Achieving this vision will require continued investment in automation, user-friendly interfaces, and workflow integration, ensuring that FAIR principles are not an added burden but a natural part of everyday research practice.

Infrastructure Development

Lowering the barrier for FAIR practice requires infrastructure that meets researchers where they already work. The priority is a workflow-native, federated architecture that plugs into instruments, ELNs, modelling environments, and analysis notebooks so that metadata capture, standardization, and deposit happen automatically. In practice, this means deployable connectors at the edge (instrument PCs, lab servers) that stream data and context directly into institutional systems (e.g., Kadi4Mat) and onward to publication platforms (e.g., Zenodo) with minimal user action, ideally “publish from the instrument” or one-click from the ELN.

A federated data infrastructure should let institutions retain control while supporting cross-site search, aggregation, and analysis. To ensure equity across the network, a shared cloud workspace preloaded with battery data toolchains, computing resources, and reproducible containers should make advanced analytics and ML accessible to small labs as well as large facilities.

Because many valuable datasets are sensitive, the stack must provide confidential computing options, fine-grained authorization, and policy-aware sharing with built-in support for Battery Passport data models where relevant. Finally, a registry of approved schemas and validators should be readily discoverable from within the tools researchers already use.

Community and Capacity Building

Technology alone won't close the data gap. People and processes must make FAIR practice effortless. The emphasis should shift from specialist training in data science or ontology development to role-appropriate, just-in-time support: short, embedded tutorials in ELNs and GUIs; recipe-style "copy/paste" templates for common experiments, and starter kits for the top battery workflows. Establishing a network of data stewards co-located with labs and modelling groups will provide hands-on help for onboarding pipelines, curating legacy data, and troubleshooting failures.

To align incentives, institutes and funders should recognize dataset releases as first-class research outputs and include data-quality milestones in grants and reviews. Industry–academia sandboxes with clear data-sharing agreements can safely unlock high-value operational datasets for method development while protecting IP and privacy. Finally, lightweight community clinics such as open office hours, hack days, validator "fix-it" sessions will help normalize rapid troubleshooting and accelerate adoption.

7.4 Forward vision

The ambition of Battery 2030+ is to create a fully integrated digital ecosystem that fundamentally changes how battery research and innovation are conducted. The goal is not to add extra tasks for researchers but to make FAIR practice implicit. Data captured during experiments, simulations, and industrial operations will flow automatically into interoperable formats, enriched with metadata and provenance, validated against community standards, and prepared for reuse with minimal human effort. The supporting tools will be embedded directly into everyday workflows—whether in the laboratory, in modelling, or within production—so that managing and publishing data becomes a natural part of scientific work.

Such an ecosystem will yield immediate and lasting impact. Routine workflows will generate predictive insights, with parameter sets and simulation outputs automatically aligned to experimental results. Researchers will be able to specify desired performance targets and receive optimized materials or cell designs derived from shared data resources. Digital twins and autonomous labs will optimize experiments in real time, while integrated lifecycle and sustainability assessments ensure that environmental and economic factors are evaluated alongside technical performance.

In the short-term (2025–2027): The priority in the near term is to embed FAIR-by-design capabilities into everyday research. Connectors for instruments, ELNs, and modelling tools will automate metadata capture and dataset submission, while baseline profiles for key formats (BDF, BPX) and AI-assisted validation will reduce the need for manual data handling. Institutional data systems such as Kadi4Mat and repositories like Zenodo will be seamlessly linked, supported by local data stewards to help researchers publish data easily and consistently.

In the medium-term (2027–2030): As the ecosystem matures, the focus will shift to federation, certification, and large-scale adoption. Institutions will join a federated data fabric enabling secure, cross-site discovery and analysis. Certification of exporters, validators, and management tools will build community trust and interoperability. Industrial and regulatory alignment—particularly with the Battery Passport—will allow the same data flows to serve both open science and compliance. By 2030, FAIR data management will be the default mode of research across Europe.

In the long-term (2030 and beyond): Beyond 2030, the European battery data ecosystem will operate as a self-sustaining, globally connected infrastructure. Automated workflows and continuous validation will make data management nearly invisible, while governance structures ensure stability, backward compatibility, and alignment with international initiatives. Supported by blended funding from public and industrial partners, this trusted ecosystem will underpin both scientific discovery and industrial competitiveness, securing Europe's leadership in the data-driven energy transition.

8.CONCLUSION

The Battery 2030+ Roadmap presents a unified and ambitious strategy to transform Europe's battery landscape across the entire value chain—from materials discovery to end-of-life recycling, and from smart functionalities to digital manufacturing and data ecosystems. By integrating seven critical research pillars—Accelerated Materials Discovery, Battery Interface Genome, Smart Functionalities/ Self-Healing Systems, New Chemistries, Digital Manufacturing & Twins, Recycling, and Data & Standardisation—this initiative lays the foundation for a battery ecosystem that is intelligent, sustainable, and globally competitive.

At its core, the Roadmap envisions a paradigm shift: from fragmented innovation to interoperable platforms; from trial-and-error development to predictive, data-driven design; and from linear production models to circular, digitally integrated lifecycles.

Strategic enablers are:

- AI-powered Materials Acceleration Platforms (MAPs) that dramatically shorten discovery cycles and link lab-scale insights to industrial relevance.
- Multiscale modelling and *operando* diagnostics that transform interface understanding into actionable design principles.
- Smart sensing and self-healing technologies that enable batteries to monitor, diagnose, and autonomously correct failure modes.
- New chemistries that unlock applications beyond lithium-ion, tailored for long-duration storage, mobility, and climate-neutral performance.
- Digital twins and modular manufacturing systems that reduce waste, improve traceability, and accelerate scale-up through real-time feedback and adaptive control.
- Advanced recycling technologies that close material loops, reduce dependency on CRMs and enable fully circular battery value chains.
- A FAIR-by-default data ecosystem that seamlessly integrates experimental, simulation, and industrial data into interoperable, reusable formats—accelerating discovery, compliance, and lifecycle optimization.

Yet, despite this momentum, Europe faces an uncomfortable reality: the gap between scientific innovation and industrial implementation remains wide. The transition from lab-scale breakthroughs to large-scale production is hindered by fragmented infrastructure, limited manufacturing capacity, and complex regulatory landscapes. The highest hurdle is not discovery, but scale, translating breakthroughs into robust, cost-effective, and sustainable industrial processes.

To overcome this, science must evolve beyond the lab—supporting engineering, standardization, and integration efforts. Collaborative platforms that unite academia and industry are essential to accelerate the uptake of promising technologies and ensure their relevance at scale. These pillars converge through shared infrastructures, harmonized standards, and coordinated regulatory alignment.

These pillars converge through shared infrastructures, harmonized standards, and coordinated regulatory alignment. The Roadmap calls for cross-sector collaboration, open innovation, and strategic investment to ensure that Europe remains at the forefront of the global energy transition.The Battery 2030+ initiative is more than a research agenda, it is a blueprint for a sovereign, sustainable, and smart battery future. By executing this Roadmap with strategic investment and cross-sector collaboration, Europe can lead the development of energy storage technologies that power not only devices and vehicles, but also climate action, industrial competitiveness, and societal resilience.

9. GLOSSARY

AE - Acoustic Emission

Advanced sensor- A sensor with enhanced capabilities to monitor properties in real time, often integrated with automated or AI-driven systems.

API - Application Programming Interface

BIG - Battery Interface Genome

BMS- Battery Management System

CEI- Cathode Electrolyte Interface

CRMs- Critical Raw Materials

CNNs- Convolutional Neural Networks

CFG -Computational Fluid Dynamics- is the use of numerical methods and algorithms to simulate the behaviour of fluids (liquids and gases) and their interactions with surfaces. It is widely applied in engineering and science to analyse flow, heat transfer, and related physical processes.

DFT methods- Density Functional Theory methods which are computational techniques used to study the electronic structure of atoms, molecules, and materials.

DoE- Design of Experiments

Direct recycling refers to a novel recycling approach for batteries, in which the high-value anode and cathode active powders and other components are recovered in whole from spent cells, with production scrap separated from each other and from the other recoverable materials.

Extended Producer Responsibility (EPR) is an environmental policy approach in which a producer's responsibility for a product is extended to the post-consumer stage of the product's life cycle.

Eco-design preparatory study for batteries provides the European Commission with a technical, environmental, and economic analysis of batteries in accordance with relevant European Directives.

Eco-design Directive provides consistent EU-wide rules for improving the environmental performance of products, such as household appliances, information and communication technologies, or engineering.

EIS- Electrochemical Impedance Spectroscopy

ESRF beamline - refers to one of the experimental stations (beamlines) at the European Synchrotron Radiation Facility- one of the world's most advanced synchrotron light sources, located in Grenoble, France.

EPR- Electron Paramagnetic Resonance

EPR – Extended Producer Responsibility

FBG- Fibre Bragg Grating- is a segment of optical fibre with a periodic variation in its core's refractive index that reflects a specific wavelength of light while transmitting others. It is widely used in telecommunications for wavelength filtering and in sensing applications to measure strain, temperature, and pressure.

HT ecosystem - High Throughout ecosystem – An AI accelerated combinatorial HT ecosystem in batteries is a coordinated environment that links automated high-throughput synthesis, characterization, simulation, and data-driven decision-making, so that new materials and battery concepts can be discovered and validated much faster.

HTE- High-Throughput Experimentation

LIB - Lithium-ion Battery

MAP- Materials Acceleration Platform

ML- Machine Learning

MOFs- Microstructured Optical Fibres

Prospective Life Cycle Assessment (LCA) is prospective when the (emerging) technology studied is in an early phase of development (e.g., small-scale production), but the technology is modelled at a future, more-developed phase (e.g., large-scale production). A prospective LCA addresses two aspects: first, the assessment of an emerging technology in an early phase of development (low TRL, e.g., lab-scale production), where the technology is modelled at a more-developed phase (high TRL, e.g., industrial-scale production) by applying upscaling techniques (also called ex-ante). Second, an emerging technology with low TRL is again upscaled to a higher TRL, but in addition, the assessment addresses a future implementation of the technology, for example with a different electric energy mix or different environmental impact effects.

QRLS- quality, reliability, lifetime, and safety

RUL- Remaining Useful Life

Re-use refers to the action or practice of using something again for its original purpose.

Re-purpose is the process by which an object with one use value is transformed or redeployed as an object with an alternative use value.

Recycle is the process of converting waste materials that are no longer functional into new materials or products.

Recovery refers to recycling processes that accomplish chemical or physical upgrading of the material to a market commodity such as cathodes or cathode precursors.

Reconditioning involves servicing, readjusting, and recalibrating materials or equipment to bring them to a near-new or original operational level.

RE- reference electrodes

SoC- State of Charge

SoH- State of Health

SoS- System of Systems - a large, complex network made up of multiple independent systems that interact and work together to achieve a higher-level function that no single system could accomplish on its own.

SIBs-Sodium-ion batteries

SSB- Solid State Batteries

SEI- Solid Electrolyte Interphase

Sustainability circle is a method for understanding and assessing sustainability and for managing projects directed towards socially sustainable outcomes.

TBMS- Thermal Battery Management System

TEM- Transmission Electron Microscopy