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This roadmap presents the transformational research ideas proposed by "BATTERY 2030+," the European large-scale research initiative for future battery chemistries. A "chemistry-neutral" roadmap to advance battery research, particularly at low technology readiness levels, is outlined, with a time horizon of more than ten years. The roadmap is centered around six themes: 1) accelerated materials discovery platform, 2) battery interface genome, with the integration of smart functionalities such as 3) sensing and 4) self-healing processes. Beyond chemistry related aspects also include crosscutting research regarding 5) manufacturability and 6) recyclability. This roadmap should be seen as an enabling complement to the global battery roadmaps which focus on expected ultrahigh battery performance, especially for the future of transport. Batteries are used in many applications and are considered to be one technology necessary to reach the climate goals. Currently the market is dominated by lithium-ion batteries, which perform well, but despite new generations coming in the near future, they will soon approach their performance limits. Without major breakthroughs, battery performance and production requirements will not be sufficient to enable the building of a climate-neutral society. Through this "chemistry neutral" approach a generic toolbox transforming the way batteries are developed, designed and manufactured, will be created.

1. Introduction

Rechargeable batteries are a key technology enabling energy storage for a vast number of applications. Batteries can accelerate the shift toward sustainable and smart mobility, help supply clean, affordable, and secure energy, and mobilize industry for a cleaner, circular economy. The transition toward a carbon neutral society and reduced net greenhouse gas emissions by at least 55% by 2030, which is the goal of the European commission,[1] requires batteries with ultra-high performance beyond their current capabilities: Energy and power density must approach theoretical limits, and outstanding lifetime and reliability as well as enhanced safety and environmental sustainability must be achieved. Furthermore, to be commercially successful, new battery technologies must be scalable, sustainable, and enable cost-effective, large-scale

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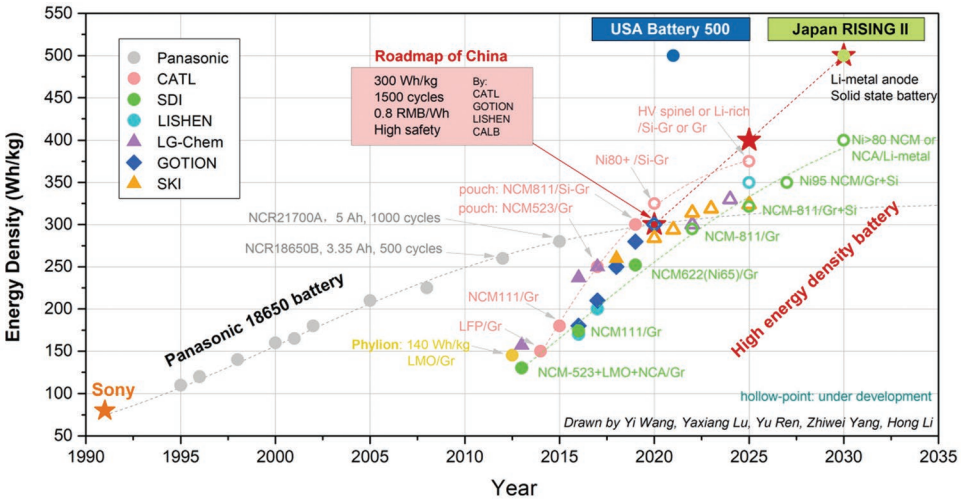

Figure 1. Comparison of the gravimetric performance of different batteries for automotive applications. The targets from the SET Plan coincide with the green line (different NCM-based generations of LIBs). Japanese Rising II follows targets similar to those of the SET Plan, while China's targets (red stars) are slightly more ambitious up to 2030. The expectations for the lithium-metal solid-state battery are the same in all roadmaps. Important to remember is that these roadmap are specifically targeting the transport sector so other battery chemistries important for other market segments are omitted. Reproduced with permission.[15] Copyright 2019 Elsevier.

production. These requirements constitute grand challenges for the battery research community which BATTERY 2030+, the large-scale and long-term European research initiative, will address. This paper summarizes the roadmap developed by the always BATTERY 2030+ consortium and is complemented by a number of articles in this special issue, including also one paper regarding the state-of-the-art.[2–11]

The market for high-energy-density rechargeable batteries is currently dominated by the lithium-ion (Li-ion) battery (LIB), which performs well in most applications and has decreased dramatically in cost. However, current generation LIBs are approaching their performance limits. Without major and cost effective breakthroughs, battery performance and production will not keep up with the developments necessary to build the climate-neutral society. While LIBs will continue to play a major role in the energy storage landscape, disruptive ideas are required that can enable the creation of the sustainable batteries of the future and lay the foundation for European competitiveness during the transition to a more electricity-based society. Consequently, there is a need to create a dynamic ecosystem that dares to include long-term, transformational research starting at fundamental technology readiness levels (TRLs) that can rapidly feed new knowledge and concepts across all TRLs as well as into commercial products. To develop the necessary breakthrough technologies, immense multi-disciplinary and cross-sectorial research efforts are needed. Europe has the potential to take the lead thanks to both thriving research and innovation (R&I) communities covering the full range of involved disciplines and well-established innovation clusters with industry. However, to realize the vision of inventing the batteries of the future in Europe, we must join forces in a coordinated, collaborative approach that unites industry, researchers, policymakers, and the public in pursuing those goals.

BATTERY 2030+ brings together important stakeholders in the field of battery R&D to work on concrete actions that support the implementation of the European Green Deal, the UN Sustainable Development Goals, as well as the European Strategic Action plan on Batteries[12] and the Strategic Energy Technology Plan (SET Plan).[13] It will allow Europe to reach or even surpass its ambitious battery performance targets set in the SET Plan), meet the strict sustainability requirements outlined by the EU,[14] and consequently foster innovation throughout the whole battery value chain.

Since its inception, BATTERY 2030+ has become an essential part of the European battery "ecosystem," addressing above-mentioned challenges with ambitious short-, mid-, and long-term objectives. These objectives are in line with roadmaps published by several associations and countries, for instance European Association for Storage of Energy (EASE), Energy Materials Industrial Research Initiative (EMIRI), European Council for Automotive R&D (EUCAR), Joint Research Centre, the European Commissions (JRC), China, Finland, India, Japan, and the USA. The performance targets of some of these roadmaps are represented in **Figure 1**.

2. Battery 2030+: A Chemistry-Neutral Approach

BATTERY 2030+ follows a chemistry-neutral approach to facilitate the invention of the batteries of the future (**Figure 2**). Its goal is not to develop a specific battery chemistry, but to create a generic toolbox for transforming the way we develop and design batteries. Thanks to its chemistry-neutral approach, BATTERY 2030+ has an impact not only on current lithium-based battery chemistries, but also on all other types of batteries. BATTERY 2030+ will join forces to focus on three overarching themes encompassing six research areas to address the key challenges in inventing the sustainable batteries of the future. These themes are summarized in the following and will be explained in more detail in Section 4:

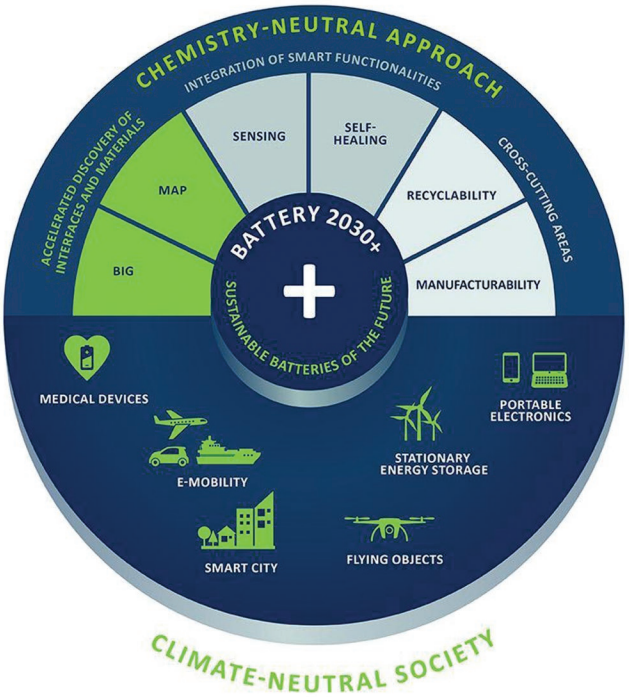

Figure 2. The BATTERY 2030+ vision is to invent the sustainable batteries of the future through a chemistry-neutral approach that will deliver ultra-high-performance batteries optimized for their intended applications, such as electro-mobility, stationary storage, medical devices, and robotics. BATTERY 2030+ proposes to focus on three main themes and six research areas that are strongly linked, all contributing new tools for accelerating battery discovery and development.

2.1. Theme I: Accelerated Discovery of Battery Interfaces and Materials

At the core of inventing the batteries of the future lies the discovery of high-performance materials and components that enable the creation of batteries with higher energy and power. BATTERY 2030+ advocates the development of a battery Materials Acceleration Platform (MAP)[16] to reinvent the way we perform battery materials research today. We will achieve this by creating an autonomous, "self-driving" laboratory for the accelerated discovery and optimization of battery materials, interfaces, and cells. This can be done by combining powerful approaches from high-throughput automated synthesis and characterization, materials and interface simulations, autonomous data analysis and data mining, as well as Artificial intelligence (AI) and machine learning (ML).

Interfaces in batteries are arguably the least understood, even though most of the critical battery reactions occur there, such as charge transfer reactions, dendrite formation, solid electrolyte interphase (SEI) formation, and cathode–electrolyte interface (CEI) formation. Building on MAP, BATTERY 2030+ proposes to develop the Batteries Interface Genome (BIG) that will establish a new basis for understanding the interfacial processes that govern the operation and functioning of every battery. The accelerated design of battery materials requires the detailed understanding and tailoring of the mechanisms governing interface formation and evolution. This involves studying the mechanisms of ion transport through interfaces and, even more challenging, visualizing the role of the electron in the interfacial reactions. These processes determine whether the ultra-high-performance batteries developed will be safe to operate and exhibit the long lifetimes that are necessary.

A central aspect will be the development of a shared European data infrastructure capable of performing the autonomous acquisition, handling, and analysis of data from all domains of the battery development cycle. Novel AI-based tools and physical models will utilize the large amounts of data gathered, with a strong emphasis on battery materials and interfaces. The data generated across different length and time scales, using a wide range of complementary approaches, including numerical simulation, autonomous high-throughput material synthesis and characterization, in-operando experiments, and device-level testing, will all contribute to new material and battery cell development.

Integrating these two research areas, BIG and MAP (BIG–MAP) will transform the way we understand and discover new battery materials and interfaces. Theme I will deliver a transformative increase in the pace of new discoveries for engineering and developing safer, longer-lived, and sustainable ultra-high-performance batteries.

2.2. Theme II: Integration of Smart Functionalities

Even the best battery will eventually fail, that is, we must develop methods that increase safety, reliability, and cycle life of batteries by introducing smart sensing and self-healing functionalities. Degenerative processes within a battery cannot be suppressed completely, and external factors such as extreme temperatures, mechanical stress, excessive power during operation, or simply ageing will, given time, act detrimentally on battery performance. From the perspectives of sustainability, economic efficiency, and reliability, new ways need to be found to increase safety and lifetime particularly in critical applications.

The BATTERY 2030+ vision is to incorporate smart sensing and self-healing functionalities into battery cells with the goals of increasing battery reliability, enhancing lifetime, improving safety, lowering the cost per kWh stored, and, finally, significantly reducing the environmental footprint.

Non-invasive sensing technologies offering both spatial and time resolution will be developed to monitor key battery cell parameters during operation and to determine defective areas or components within the cells that need to be repaired by activating/adding self-healing functions. In the battery of the future, sensors will make it possible to follow chemical and electrochemical reactions "in vivo" directly inside a battery cell during real-world operation. New sensor technologies will emerge that can diagnose the early stages of battery failure, thermal runaway, and unwanted side reactions leading to early battery ageing.

Self-healing functionalities will become an important property of future batteries in applications that require batteries with high reliability, high quality, and long lifetimes. Combining sensing and self-healing functionalities will result in batteries with a predictable lifetime and documented state of

health (SoH), state of safety, and usage history. Smart functionalities will enable better acceptance of used cells in primary and secondary applications. With its two research areas, Theme II will address the need for safe, reliable and long-lived batteries.

2.3. Theme III: Cross-Cutting Areas

The battery of the future will be designed taking into account sustainability and circular economy concepts including life cycle assessment (LCA).[17] As a consequence, considerations regarding manufacturability and recyclability are integral parts of battery R&D and must be considered at an early stage. Materials sourcing, processing, manufacturing, and assembly processes must be tailored to accommodate new chemistries and follow innovative approaches to allow for efficient remanufacturing and re-use requirements.

The manufacturability and recyclability of batteries are thus key cross-cutting areas that will develop through close collaboration between those addressing themes I and II. From the outset, new knowledge and ideas about how to manufacture and recycle batteries will inform the materials discovery and development processes.

The manufacturing of future battery technologies is addressed in this roadmap from the standpoint of the fourth industrial revolution, that is, Industry 4.0[18] and digitalization. The power of modelling and the use of AI should be exploited to deliver "digital twins"[19] for both innovative cell designs, avoiding or substantially minimizing classical trial-and-error approaches, and manufacturing methodologies.

The new materials and cell architectures envisioned in BATTERY 2030+, call for new recycling concepts, such as reconditioning or reusing active materials and electrodes. To pave the way for such a shift, material suppliers, cell and battery manufacturers, main application actors, and recyclers will be directly coupled to accommodate the constraints of recycling when developing new batteries. The discovery of new materials using BIG–MAP will integrate parameters such as recyclability, critical raw materials, and toxicity into the algorithms.

With these two research areas, Theme III will ensure that all research approaches will consider the feasibility of scaling up new materials and battery cells as well as the possibility of recycling and reusing battery components at low cost and using climate-neutral approaches.

3. Battery 2030+: A Holistic Approach

The six research areas described in three themes are interlinked, contributing new tools that will transform the way Europe discovers and develops batteries. The MAP and the Battery Interface Genome (BIG) will be powerful tools for discovering new materials and engineering battery interfaces, and in particular will be used to discover or optimize self-healing materials and chemicals. Sensors integrated at the battery cell level will provide a huge amount of data for the research community, data that will be systematically exploited by feeding the AI used in MAP. Sensing and self-healing functionalities will be strongly connected via the battery management system (BMS), which will trigger self-healing based on information from the sensors. Finally, the development performed in the cross-cutting research areas (i.e., manufacturability and recyclability) will ensure that it will be possible to efficiently manufacture and recycle next-generation battery cells incorporating new materials, engineered interfaces, sensors, and self-healing functionalities. Across these research areas, the safety and sustainability of newly developed battery technologies will be central guiding principles. The progress in all identified research areas will be essential for inventing batteries with properties that are tailor-made for their specific applications.

By following a coordinated, multidisciplinary, and harmonized approach, BATTERY 2030+ will have major impacts on the battery technology ecosystem and beyond.

3.1. Impact of a Large-Scale Battery Research Initiative

BATTERY 2030+ aims to invent the sustainable batteries of the future. More specifically, it will lay the scientific and technological foundation and provide the necessary tools to enable the next generation of high-performance, safe, and sustainable batteries. Having these novel battery technologies at our disposal will have societal and environmental impacts on many levels. It will increase energy security, reduce the environmental footprint in many application areas, and help forge a climate-neutral society while at creating new markets and jobs.

3.2. Impact Along the Battery Value Chain

The BATTERY 2030+ community will actively address the impact of scaling on energy density, that is, the reduction in weight- and volume-specific metrics when scaling from the materials level to the battery pack level. The BATTERY 2030+ themes will also address the unwanted chemical and electrochemical side reactions that reduce battery capacity over time.

Figure 3 schematically illustrates how the different components of a battery affect its overall performance. The active battery material can store a certain amount of energy per weight or volume (specific energy, 100%). As the different components of a real battery are added—for example, binders, conductive fillers, and other additives within the electrodes; current collectors, separators, electrolyte, packaging, wiring, cooling, and battery controller—the energy content per weight and volume drops, as from the storage capacity point of view a considerable quantity of "dead mass" is added. Finally, the specific energy decreases during use toward the end of life, which is defined differently for different applications.

To obtain a high-performance battery, it is necessary to start with materials having high specific energy, and to minimize losses along the manufacturing chain and during use. For novel and future battery chemistries, this is a challenge, as: (a) high-performance materials are still lacking; (b) engineering concepts have not been developed and tailored for efficient cell production; and (c) performance degradation remains an issue. The themes and research areas of BATTERY 2030+ will address these issues as shown in Figure 2.

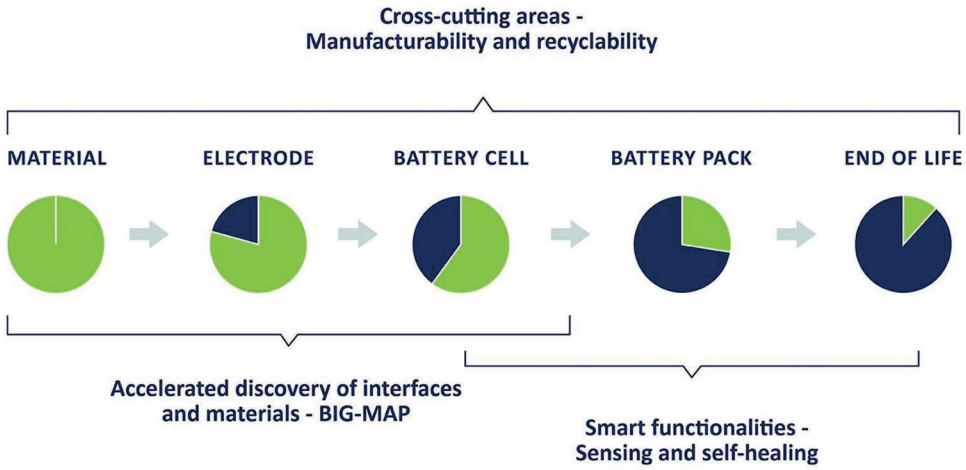

Figure 3. The decrease in total capacity as more inactive material is added when going from the material to the complete battery pack. The identified research areas will address these losses throughout the battery value chain. End of life represents the additional capacity loss due to degradation.

3.3. Impact on the Different Targets for Batteries

BATTERY 2030+ suggests actions pushing battery technologies far beyond the current state of the art. This will have an impact throughout the battery value chain by enabling and accelerating the attainment and surpassing targets in different roadmaps. The BATTERY 2030+ initiative addresses the great need for efficient and sustainable batteries. Through the activities along its three research themes, BATTERY 2030+ has an impact on several key performance indicators (KPIs) as presented in **Table 1**.

4. BATTERY 2030+: Research Areas

Battery research occurs throughout the value chain of battery development. It can be oriented toward battery cells, based on competences in chemistry, physics, materials science, modelling, characterization, etc. It can also be oriented toward systems where the battery cells are integrated into packs, to be used in different applications. Here, the field relies on knowledge of electronics, electrical engineering, systems control, modelling at the system level, AI, and ML—to mention but a few. Also, research in recycling has become more important and again relies on chemistry, metallurgy, physics, and materials science linked to the use of new efficient characterization tools.

The European research infrastructure landscape is well equipped to carry out the ideas proposed in this part of the roadmap. There are state-of-the-art high-throughput robotized material screening laboratories available in Europe as resources. Furthermore, Europe provides access to high-performance computing, the EuroHPC, and expertise within the European Materials Modelling Council. In addition, there are a number of synchrotrons and neutron facilities in Europe represented by the organizations League of European Accelerator-based Photon Sources (LEAPS) and League of Advanced Neutron Sources (LENS), which are resources with potential to enable the BIG–MAP initiative.

The areas of research advocated by BATTERY 2030+ rely on these cross- and multidisciplinary approaches with a strong wish also to integrate other areas of research to enable cross-fertilization. In this section, detailed descriptions of the research areas proposed in this roadmap are given. Each section describes the current status in the field, the challenges and expected progress in realizing the vision, and the overall objectives of BATTERY 2030+.

Table 1. Impacts of BATTERY 2030+ research areas in relation to the SET Plan targets. Dark green = high impact, lighter green = medium to lower impact.

Major impact on the SET-Plan targets						
Theme	Research Areas	Energy and power density, charging rate	Cycle life and long-lived	Reliability and safety	Environmental sustainability	Battery costs
Accelerated discovery of interfaces and materials	Materials acceleration platform (MAP)					
	Battery Interface genome (BIG)					
Integration of smart functionalities	Sensing					
	Self-healing					
Cross-cutting areas	Manufacturability					
	Recyclability					

4.1. Materials Acceleration Platform

Materials discovery and development crosscut the entire clean energy technology portfolio, ranging from energy generation, conversion, and storage to delivery and end use. Advanced materials are the foundation of nearly every clean energy innovation, particularly for emerging battery technologies. Relying on existing trial-and-error-based development processes, the discovery of novel high-performance battery materials and cell designs entails considerable effort, expense, and time—traditionally over ten years from initial discovery to commercialization. In BATTERY 2030+, we outline a radically new path for the accelerated development of ultra-high-performance, sustainable, and smart batteries, which hinges on the development of faster and more energy- and cost-effective methods of battery discovery and manufacturing.

In this section, we outline the opportunities, challenges, and perspectives connected with establishing a community-wide European battery MAP to be integrated with the BIG described below. The proposed BIG–MAP infrastructure is modular and highly versatile, in order to accommodate all emerging battery chemistries, material compositions, structures, and interfaces. Following the format of Mission Innovation: Clean Energy Materials (Innovation Challenge 6) MAP Roadmap,[16] MAP utilizes AI to integrate and orchestrate data acquisition and utilization from a number of complementary approaches and technologies, which are discussed in the sections below.

Realizing each of the core elements of the conceptual battery MAP framework entails significant innovation challenges and the development of key enabling technologies. Combined, these technologies enable a completely new battery development strategy, by facilitating the inverse design and tailoring of materials, processes, and devices. Ultimately, coupling all MAP elements will enable AI-orchestrated and fully autonomous discovery of battery materials and cells with unprecedented breakthroughs in development speed and performance.[20]

Successful integration of computational materials design, AI, modular and autonomous synthesis, robotics, and advanced characterization will lay the foundation for dramatically accelerating the traditional materials discovery process. The creation of autonomous, self-driving laboratories[21] capable of designing and synthesizing novel battery materials, and of orchestrating and interpreting experiments on the fly, will create an efficient closed-loop materials discovery process. Its implementation constitutes a quantum leap in materials design, which can be achieved only through the integration of all relevant European expertise.

4.1.1. Current Status

Conventional research strategies for the development of novel battery materials have historically relied extensively on an Edisonian (i.e., trial and error) approach, in which each step of the discovery value chain is sequentially dependent upon the successful completion of the previous step(s). While many steps of the process have been automated and integrated in part, until now, only smaller steps have been taken toward full autonomy and closed-loop discovery. For an overview of the current state of the art, please refer to Fichtner et al. in this issue.[3]

In recent years, several examples have emerged in which the close integration of virtual (typically atomic-scale) computational material design and in operando characterization[22] techniques in a circular design loop can accelerate the discovery cycle of next-generation battery technologies (**Figure 4**), such as high-capacity Li-ion cathodes[23] and materials for secondary metal–air batteries,[24] but further acceleration is needed to reach the highly ambitious goals of BATTERY 2030+. Ideally,

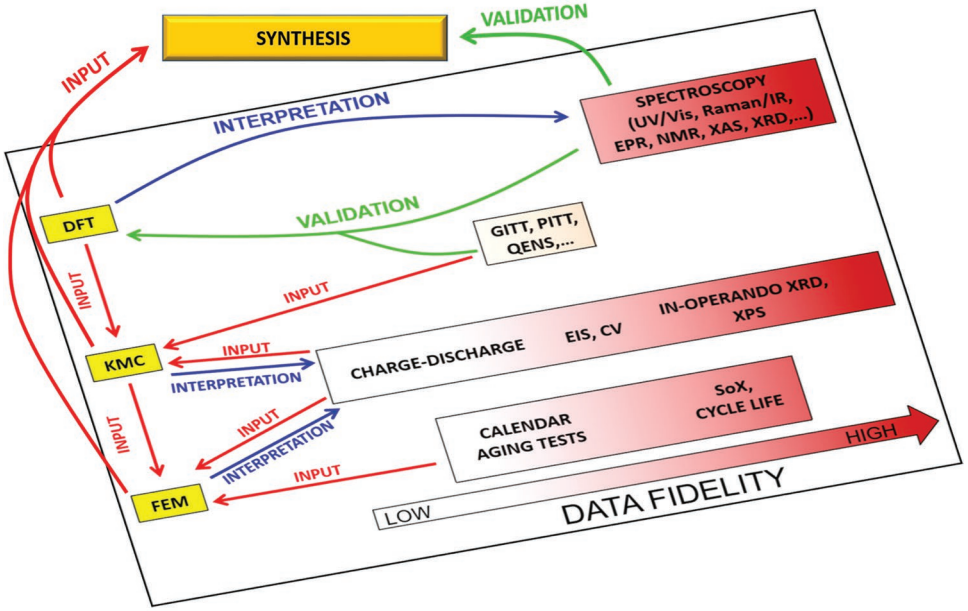

Figure 4. Illustration of the data flow between representative experimental and theoretical methods for studying battery interfaces. The fidelity of each method is generally proportional to its cost, but the fidelity–cost relationship can be optimized by acquiring data only when the given method/data is most valuable. Adapted with permission.[57] Copyright 2019, The Authors, published by Elsevier.

such a circular materials development process should integrate experimental and theoretical research in a closely coupled development autonomous platform that enables near-instantaneous cross-fertilization of the results of complementary techniques. In the following sections, we summarize the state of the art in key areas of MAP.

Interoperable data infrastructures, data management plans[25] and databases are central requirements for the accelerated rational design of battery materials and interfaces, to ensure access to and the interoperability of curated high-quality FAIR (Findable, Accessible, Interoperable, and Reusable) data[26] and multi-sourced data from different scales and domains, such as experiments, testing, and modelling. A large number of ongoing efforts in Europe and beyond aim to create extensive, flexible, and sharable databases and repositories[27,28] for experimental data. Additionally, computational infrastructures[7] such as PRACE and EuroHPC, and platforms such as UNICORE,[29,30] SimStack,[31] AiiDA,[32] and Materials Cloud[33] facilitate efficient and reliable high-throughput calculations, while only few examples like the OPTIMADE[34] REST API bridge computational and experimental data. At present, no data infrastructures exist that are capable of handling the types and quantities of heterogeneous multi-sourced data envisioned here. An overview of the potential impact of workflow technology on battery research is given in (Schaarschmidt et al. in this issue).[7] To fully exploit these data, extensive efforts, for example, by the European Materials Modelling Council (EMMC),[35] have been made to develop ontologies (e.g., EMMO), that is, common knowledge-based representation systems, to ensure interoperability between multiple scales and different techniques and domains in the discovery process.[7] A battery interface ontology BattINFO[36] is under development in Battery Interface Genome–Materials Acceleration Platform (BIG–MAP) that will facilitate the work of battery experts in different fields to convert real-life observations to a common digital representation. There are substantial efforts to establish standardized infrastructures that allow users to store, preserve, track, and share data in a curated, well-defined format that can be accessed from different platforms and for different purposes.

Multiscale modelling: Battery performance and lifetime are determined by many processes that occur on vastly different time and length scales.[37] Simulating batteries[5,7] requires insight from all of these, 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. A single computational model of virtual materials design that encompasses all these phenomena is beyond the limits of current computing power and theory, but advances in machine and deep learning models and explainable AI (XAI) provide new possibilities for autonomous parameterization and advanced multi-scaling.[38,39] Traditional single-scale models must be combined to form multi-scale workflows, for example, through generative deep learning. An overview of the potential impact of these techniques is given in (Bhowmik et al. in this issue[2]). Multi-scale modelling techniques are currently being developed, for example, to optimize real and virtual electrode microstructures[40] and to study the effects of the fabrication process on cell performance[41] and electrode surface film growth.[42]

Experimental characterization of materials and interfaces at large-scale research facilities, such as synchrotron and neutron scattering facilities, plays a critical role in ensuring sufficient acquisition of high-fidelity data describing battery materials and interfaces.[5] This calls for the ability to perform autonomous, on-the-fly analysis of the vast amounts of data generated at laboratory, synchrotron, and neutron facilities across Europe. The state of the art of the most relevant structural and spectroscopic characterization techniques related to battery materials and interfaces is discussed in detail in Section 4.3.

Autonomous synthesis robotics,[6] which can be controlled and orchestrated by a central AI, are a central element of closed-loop materials discovery. Highly automated, high-throughput syntheses are now becoming state-of-the-art for organic and pharmaceutical research,[43,44] and examples are also emerging in the development of solids, electrolytes and thin-film materials.[45–47] For energy storage materials, robotic-assisted synthesis and automation have opened the field to the high-throughput screening of functional electrolytes and active materials constituting anodes and cathodes. In combination with computational approaches such as data mining and the correlation of structure–property relationships with the performance of battery active materials, robotics has had a significant impact on the discovery of novel and promising materials.[43] A key aspect is the transformation from automation to autonomy in both synthesis and characterization.

Experimental and computational high-throughput screening of large compound libraries for activity in the accelerated formulation of relevant battery materials[6,7] via the use of automation, miniaturized assays, and large-scale data analysis can accelerate materials discovery by up to one order of magnitude, see Figure 4.[48] On the computational side, workflows have been developed to automate different steps of the calculations needed to screen for new compounds.[49] Several examples of fully automated high-throughput screening (HTS) systems for electrolyte formulation, cell assembly, and selected relevant electrochemical measurements are now available,[50] for example, at the MEET Battery Research Center in Germany.

AI in materials discovery offers great prospects,[51] but the complexity and challenges of the autonomous discovery of novel battery materials and interfaces are at a much higher scale of complexity than can be handled by existing methods. 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,[52] Phoenics,[53] and Olympus[54] have been used in prototyping applications to demonstrate key components of an autonomous, self-driving laboratory, which has not yet been achieved fully for battery applications.

4.1.2. Challenges

Availability of Curated and FAIR Data: The development of predictive models to design future batteries requires thorough validation on the basis of curated datasets with FAIR[26] data

of diverse quality (multi fidelity data). In particular, the validation of the complex models required for the inverse design[55] of battery materials and interfaces requires the integration of high-fidelity data covering complementary aspects of the material 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.

To accelerate the 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 optimization 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.[56]

While ML could potentially massively accelerate the screening and identification of, for example, the structure–property relationships of inorganic energy materials,[57] a key challenge in the discovery of battery materials and interfaces is the development of autonomous workflows (see Schaarschmidt et al.[7] in this issue) for extracting fundamental relations and knowledge from sparse datasets[58] spanning a multitude of experimental and computational time and length scales.

Challenges for Closed-Loop Materials Discovery: To ensure full integration of data from experiments and tests into MAP, autonomous protocols for data acquisition and analysis must be developed. Currently, there are few examples of automated robotics for solid-state synthesis[21,46] and, more importantly, automated approaches for characterizing battery materials and cells are either lacking or dramatically underdeveloped. Several ML based tools have recently been developed for a number of relevant characterization techniques, for example, X-ray diffraction (XRD) and X-ray absorption spectroscopy (XAS).[59,60] 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.

An important bottleneck in closed-loop discovery is the lack of robust and predictive models of key aspects of battery materials and interfaces. 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 with automated synthesis and characterization technologies will enable the envisioned breakthroughs required for the implementation of fully autonomous materials discovery.[56]

4.1.3. Advances Needed to Meet Challenges

European Strongholds: European strongholds in the battery community have always been in the forefront of the development of future battery technologies. This has resulted in a leading position regarding active materials development, the design of new liquid or solid electrolytes, development beyond LIB chemistries, as well as new experimental and computational tools to understand complex redox reactions at the heart of these electrochemical systems, to name but a few relevant areas. World-leading initiatives already exist at both the multinational level, for example, Alistore-ERI, and the national level with, for instance, the French network for electrochemical energy storage and conversion devices (RS2E), the Faraday Institution in the UK, and the CELEST and POLIS consortia in Germany, demonstrating that partnerships can be created beyond individual laboratories. The European research community is ready to support a truly European research effort dedicated to advancing our knowledge of battery materials by the creation of a European battery materials acceleration platform, combining the complementary strengths of each partner with the strongly collaborative existing environment.

Autonomous Synthesis Robotics: The comprehensive electrochemical characterization of battery materials and testing on the cell level are among the major bottlenecks slowing the development of new battery materials and interfaces.[5,7] To explore larger classes of materials in the context of specific applications, it is essential to advance the development of high-throughput synthesis robotics that address both electrolyte formulations and electrode active materials, as well as combinations thereof, both for the characterization of the materials as such and in the context of functional cells.

High-Throughput/High-Fidelity Characterization: Even though an increasing number of approaches to the high-throughput testing of battery materials is reported in the literature,[61–63] many electrochemical tests do not work on short time scales; in particular, cycling experiments can take days to months or even years.[64] To exploit the opportunities afforded by the vast number of samples, an automated high-throughput infrastructure for the in situ and in operando characterization of battery materials and cells has to be established. This infrastructure must address the issues of width and depth, and should include filtration by identified lead candidates. The combination of physics-guided data-driven modeling and data generation is required to enable the high-throughput testing of batteries and their incorporated active materials in the future, and thus to develop a battery materials platform for the accelerated discovery of new materials and interfaces.

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.[44,65] 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. The establishment of a common data infrastructure will help to ensure the interoperability and integration of experimental data and modelling in a closed-loop materials discovery process across institutions in real time. Realizing 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 decentralized 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: The root of the multi-scale challenge is that it is not known how best to couple models at different scales in an efficient and robust way.[5,7] The large gain in time and accessible size of larger-scale models generally entails the sacrifice of detail and resolution. Releasing the full potential of inverse multi-scale modelling to support new materials and device design requires radically new approaches to link scales beyond the state of the art that can be achieved by isolated research communities in individual countries.[55] ML techniques and other physics-guided, data-driven models can be used to identify the most important parameters, features, and fingerprints.[66] MAP will exploit European computational infrastructures, such as those offered by PRACE and EuroHPC, as well as the results of prior and ongoing EU and national funding efforts, for example, former and ongoing centers of excellence in HPC applications such as NOMAD and MaX.

AI Exploitation: AI-based generative models,[67] that is, probabilistic models of observed data on the spatio-temporal evolution of battery materials and interfaces, can significantly contribute to the goals of MAP, and developing hybrid physics and data-driven models will be an essential part of MAP. Currently, there are substantial gaps in the model spectrum that preclude the development of comprehensive battery models. These can be closed by AI-based techniques, but these are typically unaware and thus may violate physical laws. The key to overcoming this dilemma is the development of hybrid models in which the prediction space of AI-based models is constrained by laws of physics or in which AI is used to adapt physical models. These models must be trained on large curated datasets from advanced multi-scale computational modelling, materials databases, the literature,[68] and in operando characterization. These data must span all aspects of battery materials from synthesis to cell-level testing.[56]

Unification of Protocols: MAP will offer a unique opportunity to leverage the size of this effort in the interest of standardizing data 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 modeling, and engineering.[69] 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.

Inverse Design of Battery Materials and Interfaces: 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. Interface-specific performance metrics at different time and length scales can be achieved, while retaining a reasonable degree of control over how the interface evolves over battery lifetime.

4.1.4. Forward Vision

Autonomous BIG–MAP: Our future vision is to develop a versatile and chemistry-neutral framework capable of achieving a 5–10-fold increase in the rate of discovery of novel battery materials and interfaces. The backbone of this vision is the Battery Interface Genome–Materials Acceleration Platform (BIG–MAP), which will ultimately enable the inverse design of ultra-high-performance battery materials and interfaces/interphases, and be capable of integrating cross-cutting aspects such as sensing (Section 4.3), self-healing (Section 4.4), manufacturability (Section 4.5), and recyclability (Section 4.6) directly into the discovery process.

The full BIG–MAP will rely heavily on the direct integration of the insights developed in BIG (Section 4.2) and the novel concepts developed in the area of sensors and self-healing, which will be discussed in Sections 4.3 and 4.4.

In the Short Term: Develop a shared and interoperable data infrastructure for battery materials and interfaces, linking data from all domains of the battery discovery and development cycle. Use automated workflows to identify and pass features/parameters between different time and length scales. Develop uncertainty-based hybrid data-driven and physical models of materials and interfaces.[70]

In the Medium Term: Implement BIG in the MAP platform (BIG–MAP), capable of integrating computational modelling, autonomous synthesis robotics, and materials characterization. Successfully demonstrate the inverse design of battery materials. Directly integrate data from embedded sensors in the discovery and prediction process, for example, to orchestrate proactive self-healing.[20] Demonstrate transferability of the BIG–MAP approach to novel battery chemistries and interfaces.

In the Long Term: Establish and demonstrate full autonomy and chemistry neutrality in BIG–MAP. Integrate battery cell assembly and device-level testing. Include manufacturability and recyclability in the materials discovery process. Demonstrate five- to tenfold acceleration in the materials discovery cycle. Implement and validate a digital twin of ultra-high-throughput testing on the cell level.

4.2. Battery Interface Genome

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. Realizing this, any globally leading approach to mastering and inversely designing battery interfaces must combine the characterization of these interfaces in time as well as in space (i.e., spatio-temporal characterization) with physical and data-driven models. Thereby integrating dynamic events at multiple scales, for example, across the atomic micron scales. In this respect, we must consider studies of ion transport mechanisms through interfaces and, even more challenging, visualize 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,

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[5] is therefore key for the development of ultra-performing, smart, and sustainable batteries.

The Battery Interface Genome is inspired by the concept of descriptors in catalyst design,[71] 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 informed materials design. Identifying the multiple descriptors (or genes) for the spatio-temporal evolution of battery interfaces and interphases is a prerequisite for the inverse design process, and exceeds capabilities of conventional approaches to understanding complicated phenomena as the interrelations are complex. This requires improving the capabilities of multi-scale modelling, AI, and systematic multi-technique high-throughput characterization of battery interfaces, including in-operando characterization, to generate/collect comprehensive sets of high-fidelity data 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. 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 and radically new chemistries.

4.2.1. Current Status

Experimental and computational techniques have a challenge of being both surface and interphase sensitive. Thus, no singular technique is currently capable of providing a comprehensive description of events happening at the interface. In parallel to the development of characterization 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 interfaces upon cycling. The most prominent approach is the use of electrolyte additives that react inside the cell during initial operation, and of coatings that can passivate the surface of electrode materials and thus prevent reactivity with the electrolyte. However, many years of Edisonian trial-and-error research have demonstrated the need to use several additives working in synergy to result in an effective electrode-electrolyte interface. Accelerated development of such an interphase would greatly benefit from high-throughput techniques and the AI-assisted rationalization.

The complexity of electrochemical systems usually motivates the simplification of simulations such that they only qualitatively mimic the real situation in a battery. 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 idealized physics/chemistry-based simulations and data on real materials.[72] 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 include usually coupled multistep reactions.[73,74] These multistep reactions are often either oversimplified or the reaction steps are modelled in too ideal environments.[75] In specific cases, it is possible to combine DFT methods with classical approaches to improve the description of surface reactions,[76] but generic approaches remain limited and an efficient and systematic coupling is still lacking.

4.2.2. Challenges

Intensive efforts were made 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 analyzed in a systematic and automated/autonomous manner, to be accessible to the central BIG–MAP AI orchestrating the accelerated discovery process. To ensure meaningful synergy between experiments, simulations, and AI-based models, simulations and models need to become more realistic and include experimental conditions. Similarly, the experimental conditions should be made as reproducible and exact (i.e., ideal) as possible to decouple effects and reactions. In this regard, key challenges include the development of new multi-scale modeling concepts (including physics-aware data-driven hybrid models to identify dynamic interphase descriptors), and the development of new characterization techniques, especially in electrochemistry. Standardization of experimental data, conditions, and observables as inputs to physical models are necessary 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 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.[77] It could be envisioned that mature battery interface/interphase characterization techniques could provide high-throughput experimental input about battery interfaces during operation. One of the key challenges in establishing BIG is to automate the acquisition, curation, and analysis of the large datasets. These could feed the physics-aware data-driven hybrid models that will help to better understand and predict interfacial properties. 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 optimized laboratory-based to large-scale research-facility-based measurements and high-throughput 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[78,79] for interface/interphase development and dynamics. This has the potential to lay the foundation for the inverse design of battery interfaces/interphases,[56] for example, using region-based active learning algorithms.[80]

Understanding and tracking different types of uncertainties in the experimental and simulation methods, as well as in the ML framework of, for example, generative deep learning models,[71,81] is crucial for controlling and improving the fidelity of the predictive design of interfaces. Simultaneous utilization of data from multiple domains, including data from apparently failed experiment,[82] 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.

4.2.3. Advances Needed to Meet the Challenge

BIG offers a unique opportunity to develop a common European platform, as well as common European battery standards for data acquisition and transfer that could serve as worldwide standards. In addition to the continuous improvement and development of new experimental techniques and methodologies targeting the scale of atoms and ions, radical 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 localization, mobility, and transfer reactions. Advanced physics-based hybrid models and simulation techniques have to be used for the interpretation of cutting-edge in operando experiments. Efficient methods for using the large datasets to determine the descriptors of multi-scale/multi-structure theories have to be developed. 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.

Currently, no shared infrastructure or large-scale database of battery-oriented interface properties is available comparable to, for example, existing structure databases for organic and inorganic materials.[83] Implementing such European data infrastructure would require the further development and utilization of characterization techniques capable of providing a high-fidelity description of the interfaces and their dynamics. X-ray based techniques as well as neutron-based techniques are examples of techniques that will be critical, specifically when combined, in order to gain information about battery interfaces. Furthermore, to accelerate our findings, systematic measurements in parallel with multi-technique information/data from the same materials/interfaces must be established, representing a game-changing approach differing from the current single-technique paradigm. High-throughput experiments, should be designed to allow investigation of a large number of samples at great comparability and reproducibility alongside provision of pertinent auxiliary data. This requires workflows that can generate and analyze large amounts of data in an automated/autonomous manner, representing a major advance toward defining a new methodology for acquiring data on battery interfaces.

A key advance needed to establish BIG is the design of standardized 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. For that purpose, guidelines should be defined, becoming the project's characterization quality label. 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 standardizing 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 standardized 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. Moreover, to support the standardization of the testing protocols, platforms will be implemented and opened to European partners in order to certify the performance of batteries, helping better integrate academia and industry.

Rather than a single physical property, a multi-scale/multi-feature approach combining different computational tools will certainly be necessary to grasp the dynamics of the interface at different scales.[37] Through the use of AI-based techniques linking BIG and MAP, complex connections/features between scales that are imperceptible to humans will be recognized, and areas available for reliable predictions will be extended to new realms.

4.2.4. Forward Vision

While the traditional paradigm of trial-and-error-based sequential materials optimization starts from a known interface composition and structure, and subsequently relies on human intuition to guide the optimization to improve the performance, the forward vision is to enable inverse materials/interface design, in which one effectively inverts this process by allowing the desired performance goals to 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 inverse mapping from the desired properties to the original composition of the materials and external parameters/conditions. The generative deep-learning models (described within the MAP) represent an efficient way to optimize the data flow and build the required bridges between different domains, helping solve the biggest challenges of battery interphases (**Figure 5**). This reliance on statistical correlations renders descriptors an ideal tool for data-driven AI methods.

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 can then be reduced

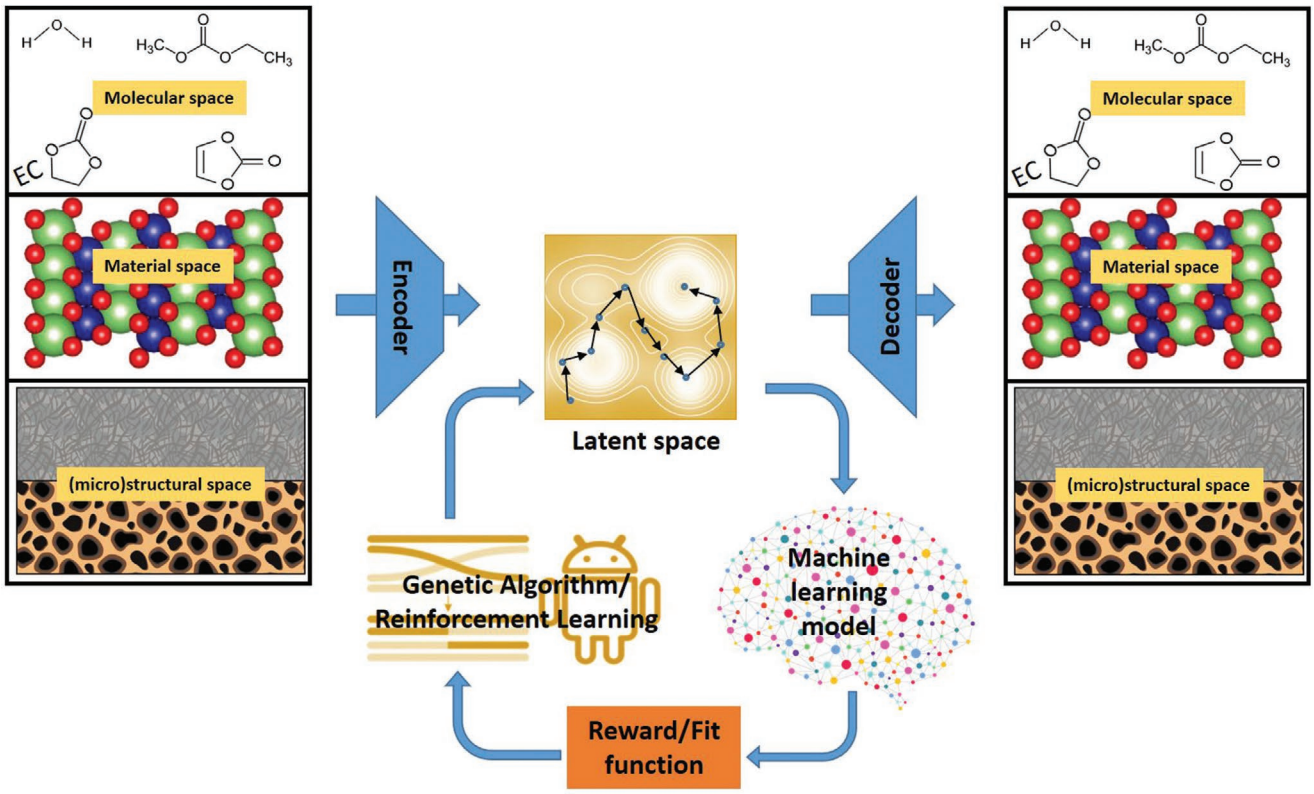

Figure 5. Generative model of interphase design. Variational auto encoder (VAE)-based encoding and decoding of chemical and structural information on a battery interphase into latent space, to enable generative battery interphase design through the use of, for example, genetic algorithms or reinforcement-learning–based exploration. Reproduced with permission.[56] Copyright 2019, Elsevier.

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 characterization, battery cell assembly, and device-level testing (BIG–MAP).

Full integration of BIG–MAP will occur step-wise, according to the following combined timeline:

In the Short Term: Establish community-wide testing protocols and data standards for battery interfaces. Develop autonomous modules and apps for on-the-fly analysis of characterization and testing data using AI and simulations.[84] Develop interoperable high-throughput and high-fidelity interface characterization approaches.

In the Medium Term: Develop predictive hybrid models for the spatio-temporal evolution of battery interfaces. Demonstrate successful inverse design of battery materials and interphases. Integrate novel experimental and computational techniques targeting the time and length scales of electron localization, mobility, and transfer reactions.

In the Long Term: Establish and demonstrate full autonomy and chemistry neutrality in the BIG–MAP platform. Demonstrate a five- to tenfold improvement in the interface performance. Demonstrate transferability of BIG to novel battery chemistries and interfaces.

4.3. Integration of Smart Functionalities: Sensing

In recent decades,[85] numerous on-board electrochemical impedance spectroscopy (EIS) devices and sophisticated BMSs have been developed to increase their quality, reliability, and life (QRL),[9] but with limited success. Although monitoring temperature, which drives reactions at battery interfaces with unpredictable kinetics, is essential for enhancing battery cycle life and longevity, this is not directly measured today at the cell level. 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, that is, fundamental science.

To challenge the existing limitations, a disruptive approach is to inject smart embedded sensing technologies and functionalities into the battery cell, capable of performing spatial and time-resolved monitoring (**Figure 6**), so that battery will no longer simply be a black box.[11]

This vision needs to be addressed at both component and full system levels and involves the possible integration and development of various sensing technologies to transmit information in and out of the cells. For that, sensors that can measure multiple parameters (such as temperature (T), pressure (P), strain (ε), electrolyte composition, electrode breathing (ΔV), and heat flow) at various locations within a cell (i.e., spatially resolved monitoring) are especially important. The target

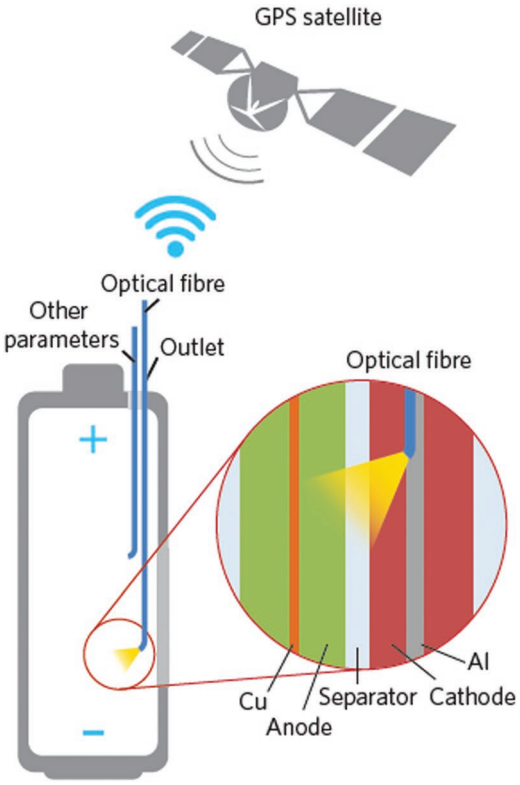

Figure 6. A future battery with an output analyzer connected to sensor (optical fibers, wires, etc.) in addition to the classical positive and negative electrodes.

is to probe the battery environment in terms of chemical reactivity and manufacturing constraints, with wireless transmission of sensing data. Lastly, and of paramount importance, is the need to identify state function estimators and to create the proper algorithms to wisely use the colossal amount of sensing data to develop intelligent responsive battery management systems.

In this section, we review the current status of sensors and sensing activities within the battery field to identify the remaining scientific, technological, and systemic challenges (see also Ref. [3] in this issue). Strategies to alleviate them are discussed and highlighted with the ultimate goal of creating highly reliable batteries with ultra-high performance and long life.

4.3.1. Current Status

Over the years, many fundamental studies have examined different battery chemistries using sophisticated diagnostic tools.[86] Although quite spectacular, these analytical techniques rely on specific equipment and cells and cannot be transferred to analyzing commercial cells. In contrast, Li-distribution density and structural effects were recently imaged in 18 650 cells, but the imaging techniques used rely mainly on large-scale facilities with limited access.[87] The need for a paradigm shift toward monitoring the battery's functional status in real time is still unmet.

Determining the state of charge (SoC) of batteries is a problematic issue nearly as old as the existence of batteries, resulting in a wide variety of ingenious monitoring approaches developed over the years (**Figure 7**). For decades, this sensing research was mainly devoted to Pb-acid technology, with the implementation of EIS to evaluate the evolution of cell resistance upon cycling in Pb-acid batteries, enabling estimation of their state of health.[88] As such, portable EIS devices have been commercialized and used in the field of transportation and telecommunications to identify faulty batteries within a module. Such devices still exist but suffer from their poor reliability (<70%). Overall, SoC monitoring remains highly challenging, and there is currently no accurate solution. Estimation of SoC today relies on a combination of direct measurements such as EIS, resistance, current pulse measurements, coulomb counting, and open circuit voltage-based estimations.

Battery-sensing activities were revitalized by the emergence of batteries in our daily lives with the emergence of novel approaches to passively monitoring the effects of temperature, pressure, strain, and ΔV of the SEI dynamic via diverse non-destructive approaches relying on the use of thermocouples, thermistors, pressure gauges, and acoustic probes. However, most of this sensing activity relies on the use of sensors outside rather than inside the battery cells, limiting the knowledge to macroscopic properties but overlooking internal chemical/physical parameters of prime importance for monitoring battery lifetime. Implantable sensors are accordingly attracting increased interest, with optical sensing being predominant (Figure 7). Recent publications have reported the positive attributes of fiber Bragg grating (FBG) sensors and other sensors for: i) accurately monitoring T, P, and ε upon cycling, ii) imaging cell temperature, and iii) estimating battery SoC without interfering with cell performance. The time has come to move out of the concept mode and solve the remaining challenges if we ever want non-invasive battery sensing to become a reality.

4.3.2. Challenges

Numerous sensing technologies for battery modules and systems have been tried (Figure 7), and challenges to embed them into practical batteries are dependent on the type of sensing technology used. Hence, knowledge of surface temperature at one location of a battery cell has long been used to validate thermal battery management system (TBMS) models using four different types of temperature sensors resistance temperature detectors (RTDs), thermally sensitive resistors (thermistors), thermocouples, and FBG optical sensors. The main limitation resides in their accuracy and the convenience with which they can be positioned within the cell.[89] Hence, while temperature contours within the cell could be plotted by implanting thermocouples within 18 650 or coin cells, drawbacks reside in the positioning of the various thermocouples and in wiring them without affecting the tightness of the cell and its performance. In contrast, hot spots can be identified within the cell using infrared thermography, but this approach suffers from poor spatial resolution together with limited temperature accuracy and susceptibility to background noise. Besides monitoring temperature, methods to sense intercalation strain and cell

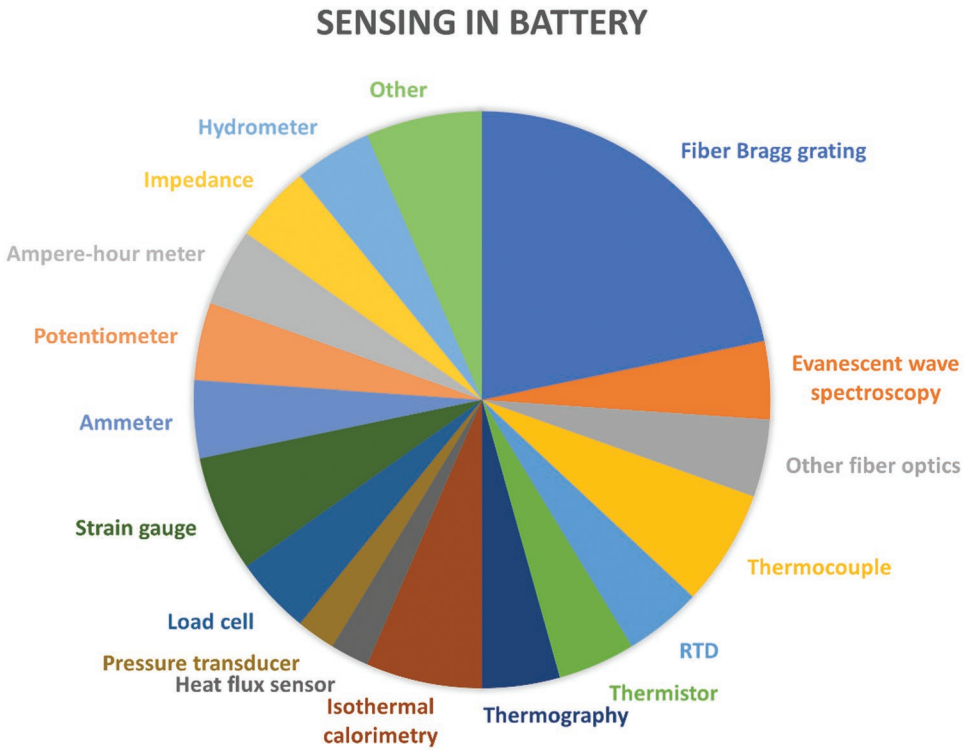

Figure 7. A glance at available sensing technologies for battery modules and systems.

pressure are equally critical techniques for monitoring the SEI dynamics that affect the SoC and SoH of batteries. Early experiments have relied on the use of in situ strain gauge measurements to probe commercial Li-ion $LiCoO_2$/C cells. Strain sensors can be used to monitor volume expansion caused by SEI growth.[90] However, the simplicity of such an approach, which relies solely on the use of external sensors, is counterbalanced by the lack of spatial information, which is critical for improving SoC and SoH batteries.

Electrochemical sensors are mainly used to sense battery chemical aspects such as SEI growth, redox shuttle species, and metal dissolution. Nevertheless, a persistent challenge in electrochemical battery diagnostics is the development of effective and (electro)chemically stable and durable (quasi-) reference electrodes (REs) that can be used in voltammetric/amperometric and/or potentiometric detection regimes. Indeed, there are difficulties in: i) having REs of well-selected chemical composition to ensure chemical inertness to the cell environment; and ii) defining the proper RE geometry and location with respect to the other cell components. The use of REs for battery sensing is therefore appealing. However, it must be realized that, as of today, reliable, user-friendly, chemically stable, long-lasting, and artefact-free cell configurations do not exist.

Optical sensors, such as FBG sensors, correlate the wavelength dependence of the emitted signal with local temperature, pressure, and strain. They are by far the most studied type of optical sensor. Few research groups have shown how FBG sensors could be used to thermally map a battery pack,[91] Li-ion pouch cells for EV applications,[92,93] or commercial 18 650 sodium-ion cells.[94] However, a difficulty with FBG use is to simply decouple pressure and temperature. Thus, the further addition of surface/ambient FBGs together with a thermal model enabled the operando monitoring of heat generated during the cell operation.[94] Furthermore, Rayleigh sensors, unlike FBGs, can provide axial resolution, in addition to be less expensive to manufacture.[95] Nevertheless, they require a more expensive interrogation system and greater calculation resources to analyze the large amount of data generated. Nano-plasmonic sensing (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). While these sensors can then be used for the in operando monitoring of physicochemical phenomena occurring on the nano scale,[96] making them requires the deposit of a metallic plasmonic nano structure on top of the fiber, whose physicochemical stability upon cycling in presence of electrolytes remains undetermined.

Finally, batteries being breathing objects that expand and contract upon cycling, "listening" to and analyzing the elastic acoustic waves generated by battery materials during operation has long been defined as potentially interesting for the study of batteries. The acoustic emission (AE) technique, previously used to monitor numerous types of battery chemistries (e.g., Pb-acid and Ni-MH) and more recently implemented in the study of LIBs during the formation stage, is very effective for studying the formatting step of batteries, detecting operation conditions leading to excessive stress and detecting the early signs of abnormal behavior that could lead to safety issues. However, AE technique suffers from some important limitations relating to the minimum threshold stress required to generate acoustic

waves and to the lack of spatial recognition.[97] Additionally, one remaining limitation of the acoustic interrogation technique is the copious wiring required to connect the acoustic transducers used for signal emission and reception.

In summary, the field of battery sensing is moving beyond proof of concept and is becoming crucial to the design and monitoring of smarter batteries. However, for this to happen, we need to master the communication between sensors and BMS systems which must be viewed as an integral part of the sensor and taken into account during the co-design of sensor and cell. Furthermore, sensor information should provoke an autonomous reaction by the BMS, which is based on proven cell and battery models and may even be AI-based. To realize the potential of this fascinating field, advances in both hardware and software are needed, which is discussed next.

4.3.2. Advances Needed to Meet the Challenges

Our proposed disruptive approach to meeting these challenges is to inject into the battery smart embedded sensing technologies and functionalities 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.

Injecting 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 successful implementation 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.

Owing to the harsh chemical nature of the battery environment, sensors with innovative chemical coatings having extremely high chemical and thermal stability must be developed. Equally, the integration of sensors in the battery will necessitate reducing their size to a few microns, to fit into the thickness of electrode separators and not affect cell performance. For manufacturing, a pressing goal is to make sensors an integral part of the battery, not simply an addition. Different strategies can be applied; for example, as done for thermistors, printing processes would create new opportunities for the integration of sensors both outside and inside battery cells as well as on battery components for in situ measurements. Moreover, an ultimate challenge is to develop wireless sensing to bypass the connectivity issues provided that the noisy environment of the battery can permit wireless communications. Indeed, adding wires to the cell could make manufacturing so expensive that it would outweigh sensor benefits. A first step toward less wiring could consist of the development of novel sensors capable of monitoring several parameters at once, for instance, coupling FBG, microstructural optical fibers (MOFs), and NPS functions on a single sensor. Similarly, different Bragg gratings could be inscribed into the same fiber to allow for so-called multiplexed measurements. Distributed sensing as offered by MOFs could be a possible solution as well, if we master their design. Lastly, cells must be used to develop sensing concepts, anticipating that findings could be implemented in modules and battery packs.

To ensure societal impact, our approach must be systematic and include the tripartite connection among battery pack, BMS, and application. Sensing will provide a colossal amount of data, which is a blessing for AI. Wise incorporation of this data into the BMS must also be considered.

4.3.3. 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 the self-healing function, would lead to a game changing approach in battery design. Needless to say, realizing this long-term vision of smart batteries includes several research facets with their own fundamental challenges and technological bottlenecks. Among the foreseen milestones are the following:

In the Short Term: At the battery cell level, develop non-invasive multi-sensing approaches relying on various sensing technologies and simple integration that will be transparent to the battery chemical environment and will offer feasible in vivo access to different relevant phenomena (e.g., interface dynamics, electrolyte degradation, dendritic growth, metals dissolution, and materials structure change). Monitor the normal/abnormal evolution of key battery parameters during cell operation and define the proper transfer functions from sensing to BMS. Increase the operational temperature window by >10% through on-the-fly sensing.

In the Medium Term: Miniaturize and integrate the identified multifunction sensing technologies at the cell level but also in real battery modules, in a cost-effective way compatible with industrial manufacturing processes. Establish new self-adapting and predictive controlled algorithms exploiting sensing data for advanced BMS. Demonstrate the reduction of electrode overvoltage in multivalent systems by >20%. Increase the accessible voltage window by >10% in Li-ion batteries.

In the Long Term: Master wireless communication between sensors and an advanced BMS relying on new AI protocols to achieve a fully operational smart battery pack. Couple sensing/monitoring advances with stimulus-activated local purpose-targeted repair mechanisms, such as self-healing, in future cell-design and chemistry generations to produce smart batteries relying on an integrated sensing–BMS–self-healing system.

4.4. Integration of Smart Functionalities: Self-Healing

The quality, reliability, lifetime, and safety (QRLS) of rechargeable battery cells are related to the electrochemical and chemical

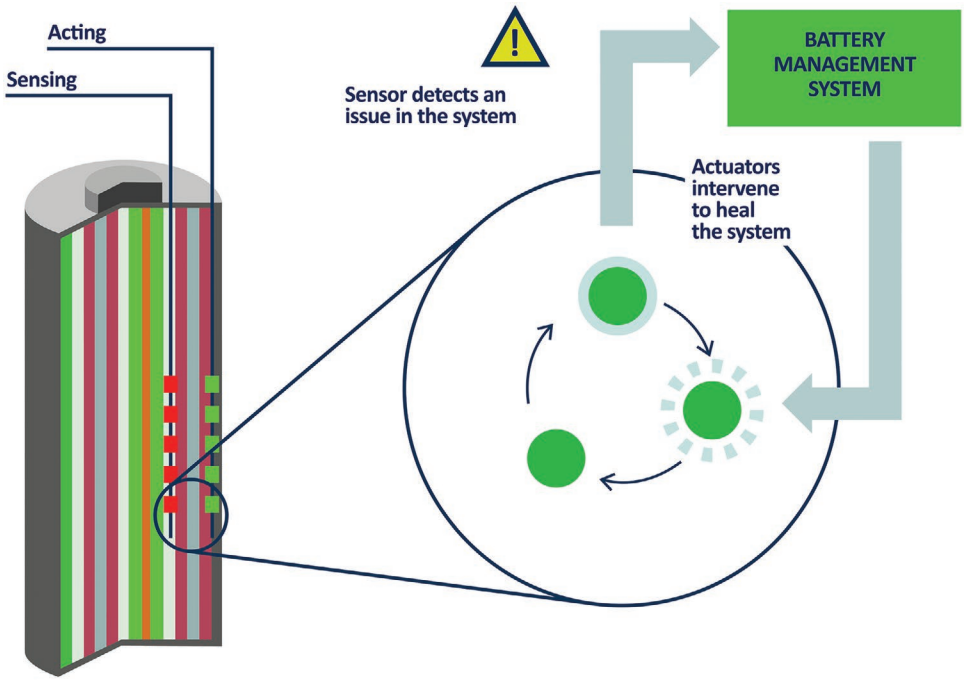

Figure 8. The synergy between sensing, BMS, and self-healing.

ageing processes present in the battery cell.[9] Detection of irreversible changes is a first step toward the improved QRLS and the cell should be able to automatically sense damage and reinstate the virgin configuration together with its entire functionality.[87] A self-healing program[9] must thus be developed hand in hand with the sensing one since they are intimately linked. The self-healing functionalities built in the cell can be autonomous (intrinsic) or non-autonomous (extrinsic),[98] both modes acting as curative actions which can significantly contribute to the QRLS of the cell. The self-healing functionalities are supplemental actions to the designed interfaces and optimized materials which are considered as preventive functionalities.

The ability to repair damage spontaneously is an important survival feature in nature and different self-healing functionalities have different kinetic, which depends on the transport of material or energy to the site of damage.[9] Can this be translated to the batteries, can we design a multi-functional self-healing without affecting cell performance in terms of energy and power density, and can this improve QRLS of the battery cells? The answers should be provided in next years. Additionally, extrinsic self-healing functionalities should be developed together with sensors and integrated into the cell/packs together with advanced BMS, where signals from the sensors are analyzed by BMS and once needed the BMS will send a signal to the actuator, triggering the stimulus of the self-healing process (**Figure 8**). This game-changing approach will maximize QRLS.

Only a limited number of self-healing approaches within the battery field have yet benefited from the general strategies and formalisms well established in nature. It is of high importance that identified self-healing tools are highly resistant to the harsh chemical environment of the cell. Copying nature's strategy, that is, relying on the use of sacrificial weak bonds for self-repair, battery scientists have developed molecules—polymers—with intrinsic self-healing properties based on dynamic supramolecular assembly, such as hydrogen bonding, electrostatic crosslinking, and host–guest or van der Waals interactions.[99,100] Functionalized and flexible polymers that are chemically compatible with battery components have been developed, with reactive species produced in the material in response to damage. Another self-healing approach, so far barely applied in the battery community, uses microcapsules hosting healing species. These need to stay active upon their release, which is triggered by a stimulus.[101] Significant advances have been achieved in the field of thermo-switchable polymers with thermal self-protection integrated into the electrolytes and current collectors.[102–104] A plethora of self-assembling materials[105–108] and bio-inspired mechanisms pertaining to the field of supramolecular chemistry and biology have also been tested to exploit radically new smart functionalities for either intrinsic or extrinsic self-healing processes.

4.4.1. Current Status

Most of the developed self-healing activities within the field of batteries have mainly targeted the auto-repair of electrodes to restore integrity of electrodes and electronic/ionic conductivity, as well as functionalizing membranes to regulate ion transport or minimize parasitic reactions. An elegant solution is use of microcapsules filled with carbon nanotubes (CNTs)[100,109] or with carbon black (CB) or with carbon-black dispersions in a combination with co-encapsulated poly-(3-hexylthiophene) (P3HT) to restore conductivity in cracked

silicon electrodes.[110,111] It was demonstrated that electronic and ionic wiring can be maintained by using a polymer coating consisting of a randomly branched hydrogen-bonding polymer that exhibited high stretch ability and sustained the mechanical self-healing repeatability[100,112,113] Another auto-repair concept[114] relies on the use of liquid metal negative electrodes, that is, a metallic alloy (Li_2Ga) having a low melting point so that the reversible liquid–solid–liquid transition of the metallic alloy can be triggered during lithiation/delithiation cycles. Thus, micro-cracks that form within the electrode can be healed during the Li-driven liquid–metal transformation.

The use of self-healing electrolytes is yet another impressive strategy to improve the electrochemical performance and durability of both non-aqueous and aqueous batteries. In a proof of concept, the strategy was used to combat the polysulfide shuttling effect in lithium–sulfur (Li–S) batteries. A self-healing electrolyte system, based on the creation of a dynamic equilibrium between the dissolution and precipitation of lithium polysulfides at the sulfur/electrolyte interface, was successfully developed and enabled high specific capacity and high coulombic efficiency.[115]

Yet other self-healing strategies are developed to minimize formation of dendrites in Li-metal batteries. Among different solutions, Ding et al. used functional metal cation additives like Cs^+ and Rb^+ [116] which enable a sustainable self-healing electrostatic shield (SHES).

4.4.2. Challenges

This brief literature review highlights that the battery community is becoming aware of the benefits that self-healing could bring to the field in terms of performance and reliability. Although this field is still in its infancy, the mentioned studies have established a basis for new research trends while stimulating novel and exciting research activities leading toward battery self-healing (BSH). Most of the reported auto-repair demonstrations are fundamentally elegant and appealing but far from practical. Such a fundamental-applied gap must be closed, and this poses numerous challenges calling for innovative research and technological development.

Main challenges are related to the most appealing degradation processes. Redox reactions occurring during battery operation are frequently accompanied by additional reactions at the thermodynamically unfavorable interface that release degradation products (i.e., dissolved transition metals or organic species from electrolyte degradation). These released metals or organic species can pass through the membrane and deposit on the anode surface or trigger the shuttling self-discharge mechanism. Therefore, it would be advantageous to functionalize the separator by anchoring to its surface chelating agents that could capture dissolved transition metal ions before they are reduced on the anode surface. Another option would be to graft proteins on the membrane to regulate the migration of parasitic organic species.

4.4.3. Advances Needed to Meet the Challenges

Different strategies can be used, some foreseen in the BATTERY 2030+ are explained more in details:

Functionalized Membrane: The use of separators for grafting/anchoring to trap molecules inside their porous channels is attractive for several reasons. i) The dissolved TM ions are transported due to diffusion and migration through the separator, rendering them available for capture by the anchored trapping molecules. ii) The porosity of the separator facilitates a high specific surface area for the deposition of an optimized number of traps per volume. The high number of ion cavity sites will increase the probability of ion capture, increasing the number of ions that can be captured per unit of volume. iii) The trapped molecules anchored inside the porous separators are far enough from the sites of electrochemical reactions that they are protected from negative/positive potentials that might affect their stability. iv) The separator provides an ideal host on which to graft molecules, which can take up ions at room temperature. v) The separator can be specifically designed with self-healing properties, like those of electrodes. Among candidates with which to synthesize the membrane, cyclodextrins turn out to be very promising. Another option, although less environmentally sustainable, is the use of crown ethers or calixarenes whose highly open structure allows the anchoring of a variety of chelating ligands capable of regulating ion transport without risk of the blockade.

Polymer Membranes: Polymer membranes are being considered as solid polymer electrolytes or as components of hybrid solid-state electrolytes. Since polymers can be formed and if needed cross-linked in situ, they can be used as mechanical healing agents within the battery cell. Moreover, they can act as a template for inorganic capsule formation on a medium time scale. With the use of composite components, the use of polymers in batteries is virtually unlimited, allowing for the development of self-healing strategies for most components and interfaces based on self-healing polymers. Polymers accordingly constitute the cornerstone of BATTERY 2030+ self-healing strategies.

Supramolecular assembly may offer a unique basis in the short term for addressing daunting challenges such as preventing the rapid decomposition of organic electrolytes, or liberating conductive self-healing materials for repairing electrodes and interfaces. Hydrogen bonding is the technique of choice to realize these possibilities, and could be used for battery components that can accommodate protic organic compounds. Similarly, ionomers can be non-covalently assembled by forming metal complexes between chains incorporating ionic chelating groups. Reversible covalent bonding (S-S) can also be used in place of non-covalent interactions, but this requires further work. Lastly, the exploration of multiphasic solid polymer electrolyte systems could also allow the application of different self-healing strategies whenever a stimulus can induce the mixing of domains.

Bio-Sourced Membrane: Another challenge is mimicking biological membranes in terms of their barrier selectivity, to control the decomposition of electrolytes so as to improve battery aging. 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 optimization of protein engineering.

Self-Healing Electrodes: The restoration of electrical properties after electrode damage is crucial in energy storage devices. As for membranes, sliding gels made of reversible bonds could be used to control the organization of the surface and to optimize the efficiency of the battery device. The main advantage of sliding gels in addition to their supramolecular interactions is the pulley effect along the polymer chain to absorb stress, permitting the reorganization of the chain architecture to return it to its initial properties. We can also use this gel as a reinforcing mechanical bandage, hence our eagerness to explore this path. Another option to explore is based on the building of composite electrodes containing microcapsules capable of releasing healing agents with the application of a stimulus, as is done in medicine with the vectorization of encapsulated medicines. Designing microcapsules with a mineral or polymeric shell, hosting Li(Na)-based sacrificial salts or other compounds that are released upon shell breaking due to a stimulus, is worth exploration.

4.4.4. Forward Vision

Ultimately, we aim to develop a system for the on-demand delivery of molecules to solubilize a resistive deposit or to restore either a defective electrode/electrolyte interface in a battery or even the conductive networks within composite electrodes. Since separators are currently a "dead" component of the battery, our strategy is to use them as our toolbox for exploring the on-demand administration of healing agents. BATTERY 2030+ will not rely solely on autonomous self-healing tools (e.g., self-healing polymers and liquid–metal alloys). It will go beyond these and include the implementation of 3D porous multifunctional material composites, capsules, supramolecular species, and polymers capable of receiving specific molecules and releasing them on demand in response to physical or chemical stimuli to repair the "tissue" constituting the electrode/electrolyte and particle/particle interfaces. The development and implementation of on-demand self-healing calls for the productive coupling of the sensing and self-healing programs within BATTERY 2030+. We hope that the use of stimuli for on-demand self-healing will open up a wide range of possibilities for realizing in vivo surgical intervention in batteries. We must be bold and open-minded to tackle these new challenges while constantly keeping in mind battery constraints in terms of the chemical environment and manufacturing.

4.5. Cross-Cutting Area: Manufacturability

Manufacturing of future battery technologies[10] is addressed in Battery 2030+ roadmap from the perspective of Industry 4.0 and digitalization, where the outcomes of the remaining chapters such as BIG–MAP, self-healing and sensorization come together in a holistic way in the manufacturing of the battery cells.[117] The power of modelling and of AI will be exploited to deliver digital twins both for innovative and breakthrough cell designs, and for manufacturing approaches, avoiding or substantially minimizing classical trial-and-error experimentation. Fully digital manufacturing analogues will allow the understanding and optimization of process parameters and of their impact on the intermediate and final product. These virtual representations can be used to manipulate and therefore actuate in the physical world, supporting greater control of battery manufacturing facilities and production lines.

4.5.1. Current Status

LIBs have become one of the main energy storage solutions[118] in most of the applications, from mobile applications to either electric vehicles or stationary applications.[119,120] Other commercial battery technologies exist (e.g., lead acid, redox flow, Na–S)[121] and new technologies are in development,[122] but LIBs will remain the driving force for electrification in the coming decade.[123] Therefore, for clarity and conciseness, we consider LIB manufacturing as a reference in this paper.

LIB manufacturing methods have been perfected on the industrial scale since the early 20th century and are well-established today. Even for the relatively new LIB chemistries, optimized manufacturing processes and giga-scale production have helped reduce cell-level costs by an order of magnitude over the last 10 years. Battery cell manufacturing[10] can generally be categorized into three phases: electrode production, cell assembly, and cell finishing. The electrode productions phase comprises several steps, such as mixing, coating, drying, slitting, calendaring,[124] the coating and drying steps being the most cost-intensive processes.[125] While in the cell assembly phase, steps such as stacking and electrolyte filling are becoming critical, because in general they are the most time and economy consuming. Finally, in the cell finishing phase, formation and ageing of the cells are the most cost-intensive processes, reflecting the challenges of processing time and yield rate.

Despite this well organized and efficient sequence, current approaches to accelerate the model-based cell design[126,127] for one hand and model-based battery manufacturing[128–135] for the other hand, still need to be adapted to meet the needs of a rapidly growing and constantly evolving battery technology landscape. Thus, modern battery manufacturing processes should be designed with the following goals in mind:

- Accelerate new cell designs in terms of performance, efficiency, and sustainability. Mechanistic models where the critical steps of the formation and ageing should be covered and their coupling with advanced optimization algorithms within AI frameworks, will facilitate inverse electrode and cell design. This approach would represent a crucial step toward autonomous battery design discovery and optimization, as it connects the desired properties to specific cell configurations, electrode compositions, and material structures as targets to manufacture, characterize, and test (**Figure 9**).
- Accelerate the optimization of existing and future manufacturing processes in terms of cell chemistry, manufacturing costs, and sustainability/environmental impact. By building computationally efficient and accurate digital twins of the manufacturing process (**Figure 10**), addressing not only the

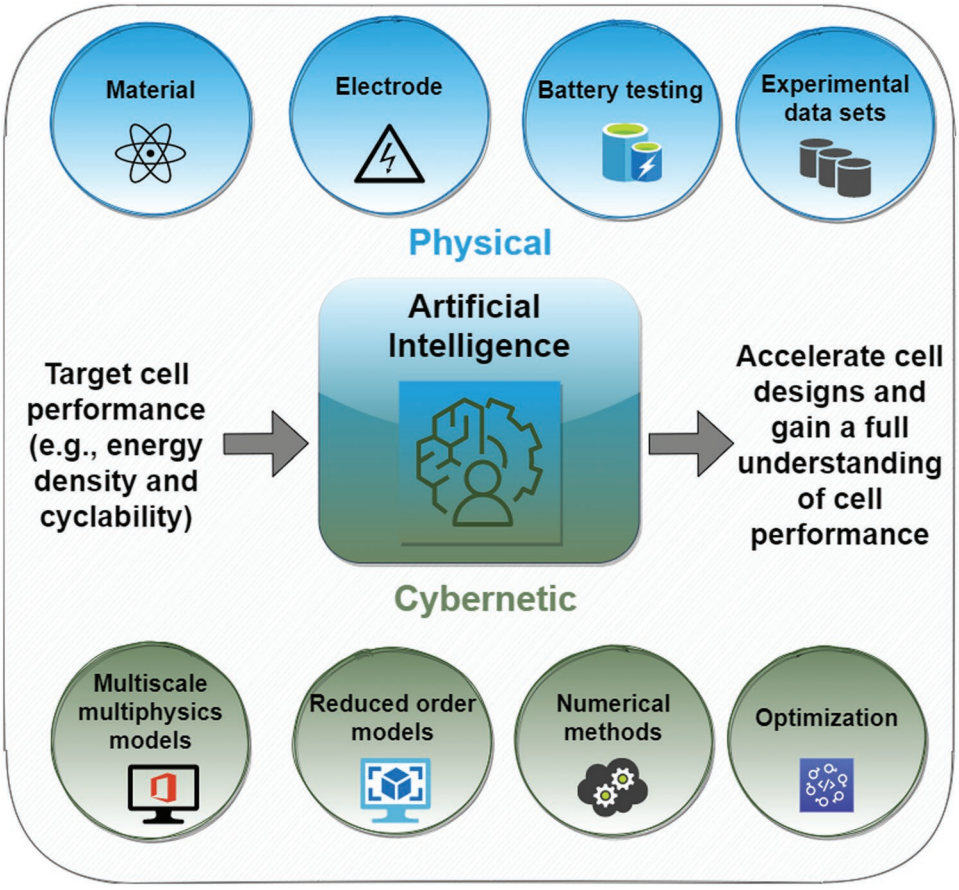

Figure 9. Inverse cell design based on digital twin of a cell.

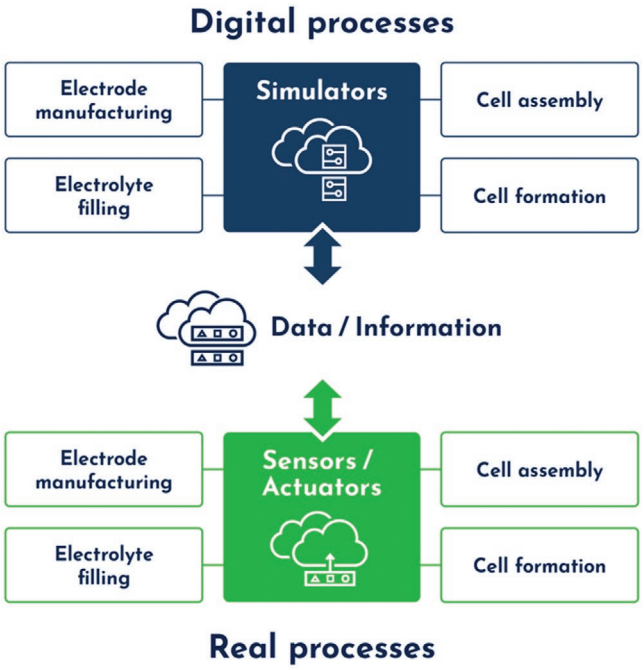

Figure 10. Digital twin of cell manufacturing processes.

multiphysics but also numerical approaches will facilitate to meet the target efficiently.

- Close the loop between cell design and cell manufacturing development, where cell performance and ageing aspect could be taken into account prior to the manufacturing phase. Thus, a holistic digital twin covering the whole battery cell manufacturing chain, from materials to cell usage aspects will promote sustainable, efficient manner of manufacturing battery cells.

New concepts will include radically new designs to minimize scrap and primary energy use and to produce sustainable products. In this regard, current multiphysics modeling can be of great importance in battery design and manufacturing. However, more effort is needed to develop a multi-scale physico-chemical computational platform coupled to AI algorithms for the full manufacturing process chain of LIBs.

4.5.2. Challenges

Current LIB manufacturing processes face numerous challenges to meet highest standards on quality, low environmental impact, and economic competitiveness. Given the disruptive nature of the concepts to be developed within the

BATTERY 2030+ initiative, there is also the need to think outside the box in cell design and manufacturing fields. The manufacturability roadmap will therefore focus on providing methodology to develop beyond state-of-the-art processes in the future.

The challenges faced by the battery manufacturing value chain can be divided into two levels. The first level of challenges is related to general methodologies for current battery production with a strong impact in the short term, but this will continue challenging the manufacturing of future battery technologies. The second level involves advanced manufacturing concepts and approaches for future battery technologies that are on our technological horizon. This is at the core of the scope of BATTERY 2030+ and is central to this roadmap. According to these two levels, the following challenges may be outlined:

a) Manufacturing challenges associated with current (mostly Li-ion) battery manufacturing technologies

First, it will be necessary to overcome today's use of trial-and-error approach as a general tool to fine-tune current battery manufacturing processes to shorten development time. The current process chain is highly complex, and it has associated very high investments. In this line, a competitive production requires the exploitation of economies of scale, which leads to so-called gigafactories, with tens of GWh of manufacturing capacity. These factories are usually very specialized in terms of battery chemistries and limited to a few cell formats, which makes the introduction of new chemistries and materials, as well as the manufacturing of novel cell formats, very challenging and associated with high start-up costs and material waste. For this reason, the production of small series for special applications, with a few tens of thousands of cells, is very difficult and expensive, limiting the market launch of novel materials and chemistries. On the other hand, it is worth mentioning that despite the strong optimization of current production lines, very large quantities of materials and cells still do not comply with specifications.

All in all, it is clear there are several difficulties in adapting/modifying current manufacturing processes to accommodate next-generation batteries and innovations, such as those relying in the use of metal foil electrode (negative electodes) (e.g., metallic lithium) and solid electrolytes (e.g., polymer, hybrid, or inorganic). To overcome these difficulties, we need to develop tools for predicting the impact of processing parameters on the characteristics and performance of the final product—or, otherwise, to predict the optimum processing parameters given the characteristics of starting materials—to leave behind trial-and-error, as stated in the state-of-the-art section.

Furthermore, to limit the material waste in manufacturing processes, we need to establish manufacturing processes allowing for component-level recycling/reuse (e.g., electrode recovery and reuse from end-of-life well-performing cells). This scrapping reduction together with the use of less solvent and energy, and faster manufacturing, especially during the formation step, will lead to a general reduction of process costs.

b) Challenges related to future battery materials and technologies arising as a result of the foreseen highly innovative battery R&D scenario

There is a need for a flexible manufacturing process design strategy, as shown in recent projects within the in the framework of the BATTERY 2030+ (i.e., BIG–MAP, BAT4EVER, HIDDEN, INSTABAT, SENSIBAT, SPARTACUS) that will produce innovative materials/interfaces, self-healing materials and sensors with specific manufacturing demands. Also, rapid and sustainable prototyping methods will be needed to implement the design rules from BIG–MAP. In addition, the introduction of self-healing materials/sensors plus their potential need for external physical connections at the cell level will require activation/bi-directional communication that will impact on the cell design and cell manufacturing activities. Design rules will also be needed for these sensors from the production point of view, addressing scalability, automated integration, cost, and recyclability.

In other terms, the introduction and viable upscaling of additive manufacturing or other mesoscale composite materials in electrode and cell processing, without affecting microstructure/functionality, will generate a need to preserve textural/functional properties.

In any case, efficient and accurate tools to predict the impact of any time of manufacturing parameters on the functional properties of battery components will be needed, partly in parallel with the introduction of new materials and concepts at the cell level.

Finally, there is a need for new manufacturing routes facilitating direct recycling methods that preserve the structural elements of the cell (e.g., electrodes and sensors).

4.5.3. Advances Needed to Meet the Challenges

Considering the challenges stated in the previous section, the advances needed for future cell manufacturing processes can be summarized as follows:

- A digital twin for inverse cell design, predicting disruptive cell designs capable of meeting performance targets (e.g., for energy, power, and cyclability).
- Flexible and scalable manufacturing processes, as well as flexible, high-precision modelling tools for the optimization of processing conditions and machine parameters; as well as real-time models for the processing of produced electrode data including their performance in the cell (i.e., a digital twin of cell manufacturing) to minimize human labor, trial and error and waste products.
- Validated multiphysics and multi-scale models coupled to AI algorithms of cell manufacturing processes capable of providing an accurate understanding of each step of the process.
- A complete digital twin of the manufacturing process including cell design and geometry aspects.

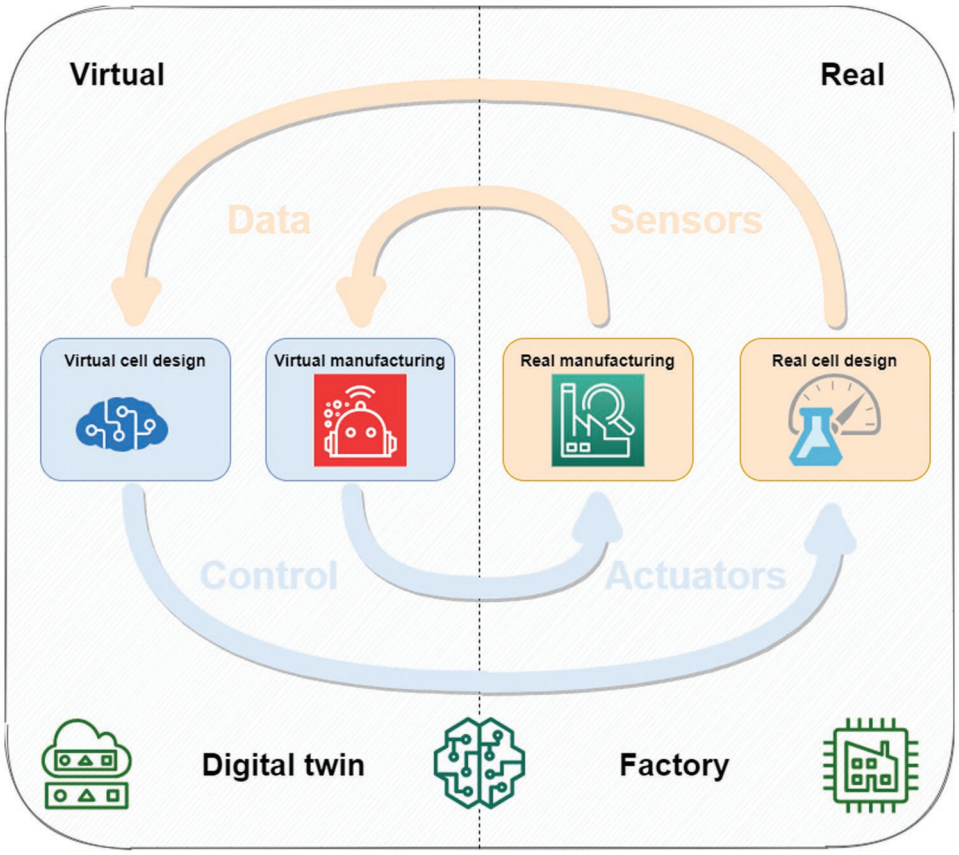

Figure 11. AI-driven design and manufacturing methodologies linked together as a whole.

4.5.4. Forward Vision

The main goal of the digital twin models designed for cell manufacturing processes is to resolve physical issues faster by detecting them earlier in the real process, and to predict outcomes with a much higher degree of accuracy (Figure 10). Additionally, their ability to evaluate the performance of equipment in real time may help companies obtain value and benefits iteratively and faster than ever before.

The implementation of these techniques and methodologies calls for sequential step-by-step development in the short, medium, and long terms. Central to this process is the development of physical modelling tools as a source of data feedstock for AI tools.

In the long term, that is, ten or more years, full maturity of the methodology is expected, closing the loop by means of integrating the cell design and manufacturing design sub-loops, interfacing with the outcomes of the BIG–MAP and smart functionalities (sensors and self-healing) to form a fully autonomous system (using AI) (see **Figure 11**). In addition, some parts of this methodology can be progressively made available to the industry, before the full package becomes available as a commodity in a new state of the art.

In the Short Term: The approach will be implemented starting from the state-of-the-art information, and it will be focused on the battery cell design methodology. This will include the improvement of simulation tools, such as multiphysics models, with the goal of reducing the computational burden and implementing current AI techniques, through ML methods, for cell design and to the LIB manufacturing steps. Additionally, the improvement and up-scaling of new manufacturing processes (e.g., 3D printing and dry processing) are also foreseen.

In the Medium Term: A proof of concept of a digital twin of a LIB cell design, as well as a proof of concept of a cell manufacturing process are expected. Inputs from other research areas coming from BIG–MAP, sensing, self-healing and recycling will be integrated into the process. The methodology will be adapted to the manufacturability of new battery technologies with the launch and implementation of the AI-driven methods for manufacturing, after developments in cell-level design and in new innovative manufacturing processes. This can then be used for the development of scalable battery chemistries, for example, multi-valent and organic battery chemistries. This can also be to demonstrate the transferability of the established BIG–MAP concept to alternative battery concepts.

In the Long Term: The overall AI-driven methodology will reach full maturity and implementation, by integrating cell design sub-loops that converge in holistic prototype development, forming a fully autonomous system supported by BIG–MAP. This methodology developed as a commodity, which will also contribute to the foundation of a new state of the art, will be progressively deployed to industry and academia.

4.6. Cross-Cutting Area: Recyclability

New materials, interfaces/interphases, and cell architectures call for new recycling concepts,[11] such as reconditioning or reusing electrodes. Industrial participation will be brought on board early. 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: 1) design for sustainability (including eco-design and economic and social aspects considering the whole life cycle), 2) design for dismantling, and 3) design for recycling approaches. In such a way, a circular economy is addressed with reduced waste, small CO_2 footprint, and more intelligent use of strategic resources.

Implementation of 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).

4.6.1. Current Status

The battery recycling industry has developed significantly in the EU since the implementation of the Batteries Directive (Directive 2006/66/EC),[136] which introduced extended producer responsibility (EPR) for battery waste. The Directive forces battery producers, or third parties acting on their behalf, to finance the net cost of collecting, treating, and recycling waste batteries. The EPR concept is aimed at promoting the integration of the environmental costs associated with goods throughout their life cycles into the market price of the products. In addition, the EU has issued a number of supporting and guidance documents as well as the recycling efficiency regulation, specifying minimum requirements for battery recycling processes, according to the battery chemistries. According to this regulation, the recycled content should reach: 65% by weight for lead-acid batteries, 75% by weight for nickel cadmium batteries, and 50% by weight for all other batteries. A revision of the Battery Directive is expected to be published by 2021 with updated categories and recycling efficiencies.

Currently, pyrometallurgy is the most applied method. After potential dismantling and sorting into categories according to the 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 12**.

4.6.2. Challenges

The development of closed material loops in the interest of a circular economy will be required to ensure the security of supply after the ramp-up phase of the battery market. Innovative collection, processing, and recycling technologies to be developed will be needed for the recovery of not only valuable elements but of all cell components to increase sustainability, which is also considered in the new draft of the battery directive.

The definition and implementation of design for sustainability for future batteries/cells will provide market advantages for European manufacturers and embed their products in closed loops. Closed loops will also decrease the dependency of the EU on critical metal imports.

Life cycle thinking, encompassing resource extraction, manufacturability, the use phase, and reuse/recycling, needs to be integrated into the design phase of new battery systems

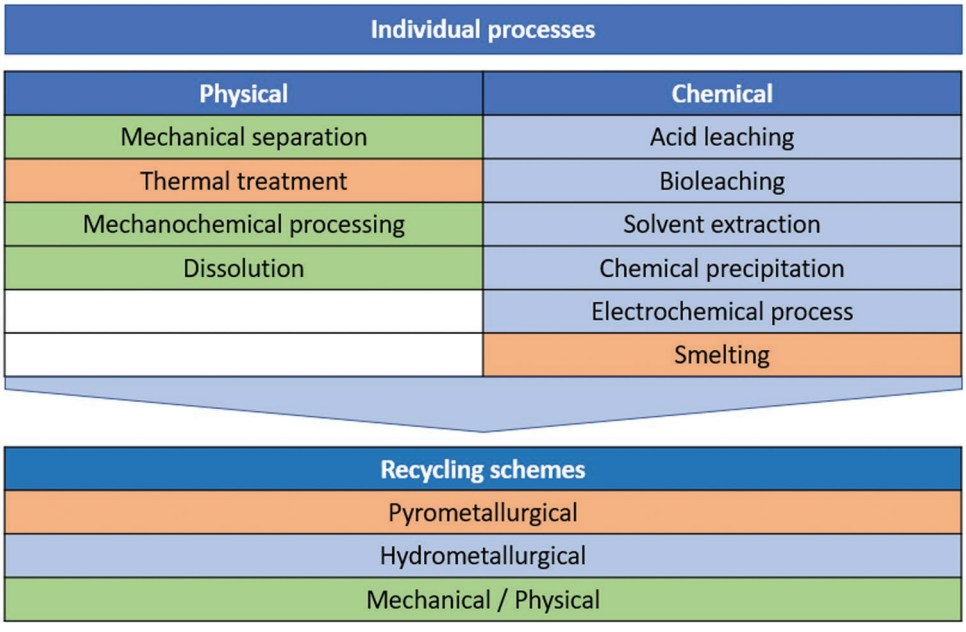

Figure 12. Recycling processes and schemes.

to increase their overall sustainability. In the following, current challenges as well as challenges foreseen for the medium and long terms are listed.

Specific short/medium-term challenges:

- The number of battery chemistries on the market is increasing. Multiple Li-ion chemistries will make specific recycling processes more difficult, and sorting quality will become a major challenge to overcome in order to have specific processes applicable to component recovery.[137] Standards for identification are important on the battery and cell levels in order to overcome these challenges.
- New battery technologies seem likely to enter future markets, for example, solid-state, lithium-sulfur, redox flow, and metal-air batteries in mobility and stationary applications. Proposed new recycling processes to cope with all these chemistries (and related BMS) will create new process challenges; for example, the presence of Li metal will affect safety aspects of the recycling processes.[138] Recycling processes may have to be redesigned, for example, to use an inert gas atmosphere, depending on the battery type.
- While the transition to aqueous processing of electrodes on the large scale is inevitable with regard to economic and ecologic improvements in battery manufacturing, the same relevance of this transition accounts for recycling and recovery processes of electrodes.[139–141] Obsolete binders and additives will have to be removed in advance to further recovery steps of active materials.[142,143]
- Despite recent progress regarding direct recovery of electrode active materials,[144,145] an additional upscaling of electrode chemistries will be necessary in many cases, as decommissioned batteries will likely contain outdated electrode chemistries. Although first results have been published, for example, the upscaling of LCO to $LiNi_{1/3}Mn_{1/3}Co_{1/3}O_2$,[146] this represents one of the major challenges to be tackled within the next few years.
- Several recycling processes are likely to cause impurities in directly recovered electrodes such as aluminum or copper fragments from the current collectors.[147] Even though such impurities can be beneficial in some cases,[148] generally, these direct recycling specific aspects need to be overcome to obtain reusable and competitive electrodes.
- Following the large quantities of EV batteries available on the market, new business cases are appearing, for example, the reuse of battery modules or cells after sorting to provide a longer service life or a second life. As a result, the batteries eventually coming to final recycling can be expected to be at a more advanced degradation stage and in a more mixed condition. In addition, although desired, global battery standardization cannot be expected given the multiple applications on the market, so chemistry identification and quality sorting will become even more challenging. In near future, decommissioned batteries will not provide sufficient information about cell chemistry and electrode condition to handle their recycling in an ideal way, which is why fast analytical measures like lithium content determination in cathodes have to be implemented.[149] The required level of expertise can only be expected if advanced AI development and novel tracer technologies, for example, marker particles with magnetic codes,[150] complement more traditional recognition means such as labelling and visual observation.
- The amount of information associated with batteries will increase, first through more and more sophisticated BMS, then possibly at the local level with information from sensors. Processes to handle information from these innovations during the recycling phases will have to be developed and standardized. Such advanced data will provide valuable input for second-life applications and options to exchange individual aged battery cells in a battery pack.
- The huge amounts of battery systems/modules to be recycled will require enormous logistical efforts, and transportation of these systems/modules will significantly increase costs, safety issues, and the CO_2 footprint. Novel decentralized collection and recycling processes/units need to be established, and societal acceptance issues need to be considered.
- A legislative framework must be established to foster/safeguard sustainable design, including design for recycling.

Tentative longer-term challenges

- Large volumes of spent batteries will require the transformation of recycling plants and a move to highly automated processes from sorting and dismantling down to the recycling itself. Generation 4.0 recycling plants will call for major investments. Innovation will be needed to demonstrate highly flexible but economically feasible processes for all the steps of recycling, enabling the treatment of multiple sources of batteries with potentially different chemistries.
- The recycling technologies will need to recover future intelligent battery components such as sensors, self-healing components, and any kind of information-linked components.
- Additional circular economy business ecosystems for reconditioning and/or reusing recycling products/materials will have to be developed and located near battery recycling units (decentralized, if possible).

4.6.3. Advances Needed to Meet the Challenges

To meet the challenges, it is necessary to establish a new recycling model based on data collection and analysis, automated pack disassembly to the cell level, investigating reuse and repurposing whenever possible, automated cell disassembly to maximize the number of individualized components. In addition, it is important to support the development of selective powder-recovery technologies that recondition powders to battery-grade active materials that are reusable in batteries for automotive/stationary applications with significantly reduced logistical efforts.

The present "Eco-design preparatory study for Batteries"[151] has the goal of providing the European Commission with a technical, environmental, and economic analysis of batteries in accordance with relevant European Directives, especially

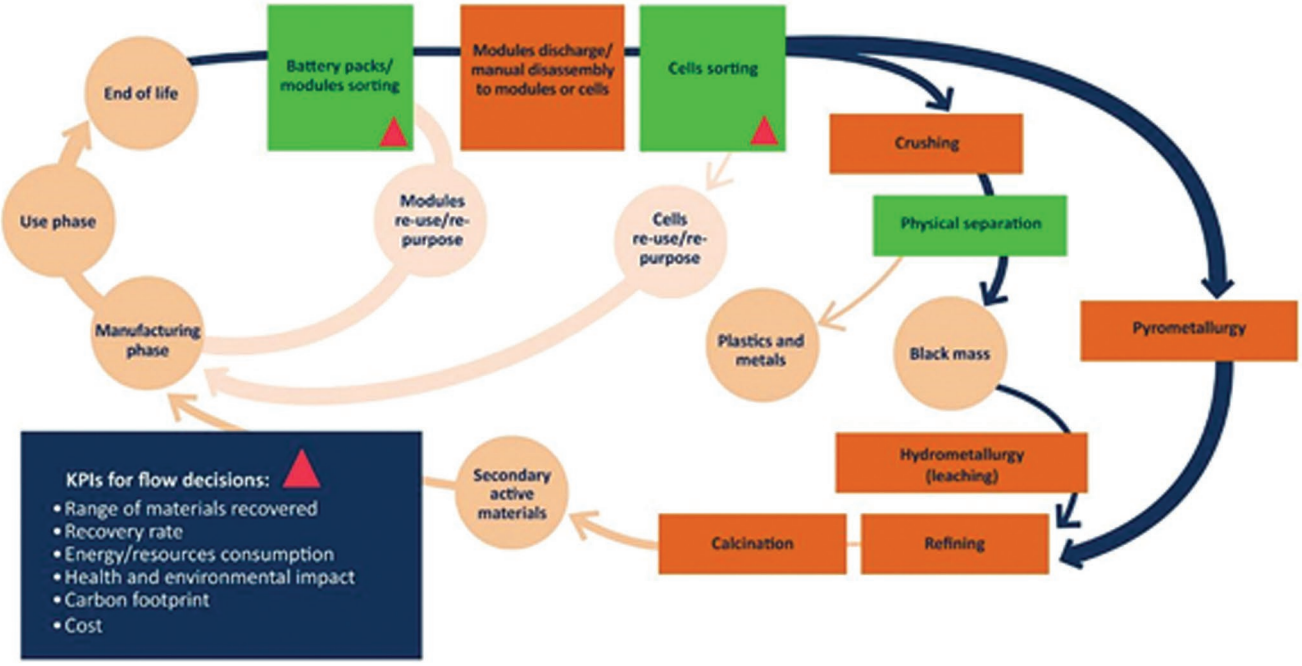

Figure 13. Present recycling process.

the Eco-design Directive (2009/125/EC).[152] Sustainability is addressed within this description, but social aspects are not considered. Moreover, the outcome of the study considered only a limited number of chemistries and application fields. In contrast to the "Eco-design preparatory study for Batteries," not only technical, environmental, and economic aspects should be considered, but also social aspects to ensure sustainability. Furthermore, the proposed approach has to be technology neutral to accommodate any innovative developments.

The proposed approach aims to provide a basis for holistic sustainable battery design starting from raw and advanced materials, design for manufacturing, and material recycling. It will provide criteria and requirements for BIG–MAP and sensing functionalities to enable high-efficiency recycling to recover critical raw materials and minimize the carbon footprint. The focus is not only on the use phase, but on the whole life cycle (i.e., life cycle sustainability) by means of prospective LCA,[153] contributing by defining rules and standards for the recycling part of the loop.

In respect of future developments, it is necessary to develop a ground-breaking new recycling process compared with the current state of the art. The current recycling flow, through pyro and hydro processes encompassing multi-processing steps, is summarized as shown in **Figure 13**. Considering the increasing variety of battery designs and chemistries, as well as the technological readiness, a multilateral approach to battery recycling consisting of pyro and hydro processes, as well as direct recycling methods will dominate the next decade.[154] However, in light of sustainability, an increased focus on direct recycling methods, where not only the most valuable but all components are recovered, is inevitable. Furthermore, the dependence of hydro and especially pyro processes on the market value of metals like cobalt and nickel will result in higher economic volatilities and less planning reliability.[155]

Based on a novel integrated approach to recycling designed materials (as developed in BIG–MAP, Battery 2030+) and sensor technologies, new models should be developed (**Figure 14**) based on:

- data collection and analysis (e.g., from labels, BMS, and sensors)
- modern small-carbon-footprint logistics concepts, including decentralized processing
- automated pack disassembly to the cell level
- investigating reuse and repurposing wherever possible
- automated cell disassembly to maximize the number of individual components
- development of selective technologies for powder recovery and powder reconditioning to battery-grade active materials reusable in batteries for automotive/stationary applications
- international collaboration to be stimulated and developed

4.6.4. Forward Vision

The new recycling process will be the basis of a series of R&I actions with the main purpose of implementing direct recycling in the long term (see **Figure 15**).

If the materials/components are not suitable to be reconditioned to battery grade because of, for example, structural or purity constraints, a fall-back alternative in the last stage of the new process could be to convert them to precursors with a view to eventual changes of composition ratios, anticipating future chemistry changes and new-generation materials.

In the Short Term: Start integrating design for sustainability and dismantling, develop a system for data collection and

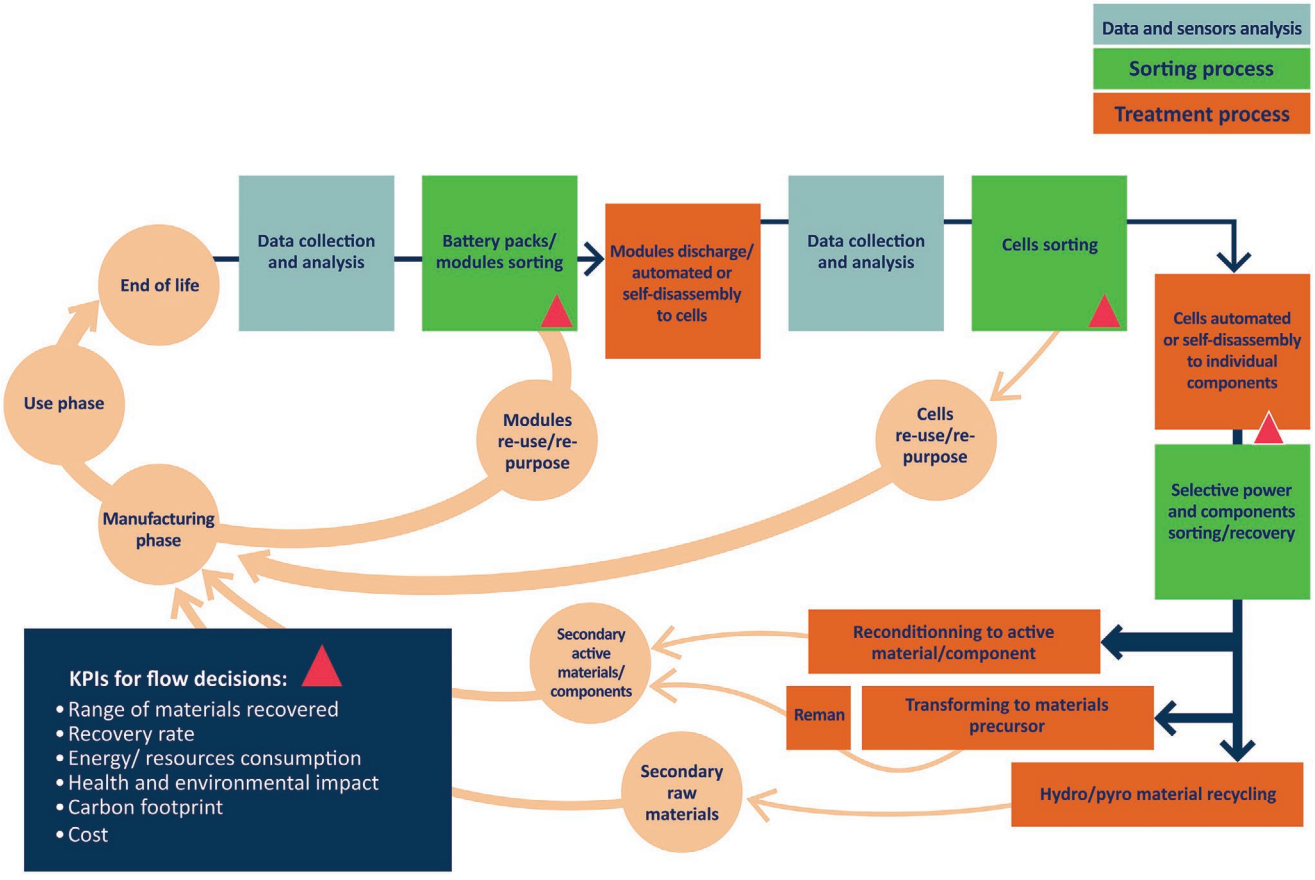

Figure 14. Future recycling process: direct recycling fully integrated with reuse.

analysis, start-to-end traceability, develop technologies for battery pack/module sorting and reuse/repurposing, and start developing the automated disassembly of battery cells. Develop new tests for rapid cell characterization.

In the Medium Term: Develop the automated disassembly of cells into individual components, as well as sorting and recovery technologies for powders and components and their reconditioning to new active battery-grade materials. Test recovered materials in battery applications. Develop prediction and modelling tools for the reuse of materials in secondary applications. Significantly improve, relative to current processes, the recovery rate of critical raw materials (e.g., graphite recovery) as well as energy and resource consumption.

In the Long Term: Develop and qualify a full system for direct recycling; the system should be economical, viable, safe, environmentally friendly, and have a smaller carbon footprint than current processes.

5. Summary

Europe is presently creating a strong battery research and innovation ecosystem community where BATTERY 2030+ has the role to provide a roadmap for long-term research for future battery technologies. LIBs still dominate the market for high-energy-density rechargeable batteries. However, current generation LIBs are approaching their performance limits despite new generations coming in near time. The transition toward a zero-carbon emission society calls for the development of batteries with higher performance, with respect to both energy and power density. Future batteries must have an improved ecological footprint. They will be characterized by outstanding lifetime and reliability as well as enhanced safety and environmental sustainability. This will most likely demand batteries approaching their theoretical limits.

With this roadmap we aim to contribute to the development of a dynamic European ecosystem that fosters long-term, transformational research starting at fundamental TRLs gradually forming the basis for novel concepts and technologies that later can be transformed into products. To develop the required breakthrough technologies, we strongly believe in multi-disciplinary and cross-sectorial research efforts across the European battery community. BATTERY 2030+ has developed a chemistry-neutral approach to facilitate the invention of the batteries of the future. We create a generic toolbox transforming the way we develop, design, and manufacture batteries, which later branch out into the development of specific battery chemistries and technologies. In pursuit of this approach, we strive to develop capabilities for diverse battery technologies and build synergies in our understanding. In order to accelerate progress, we have identified three cross-cutting themes that shall be

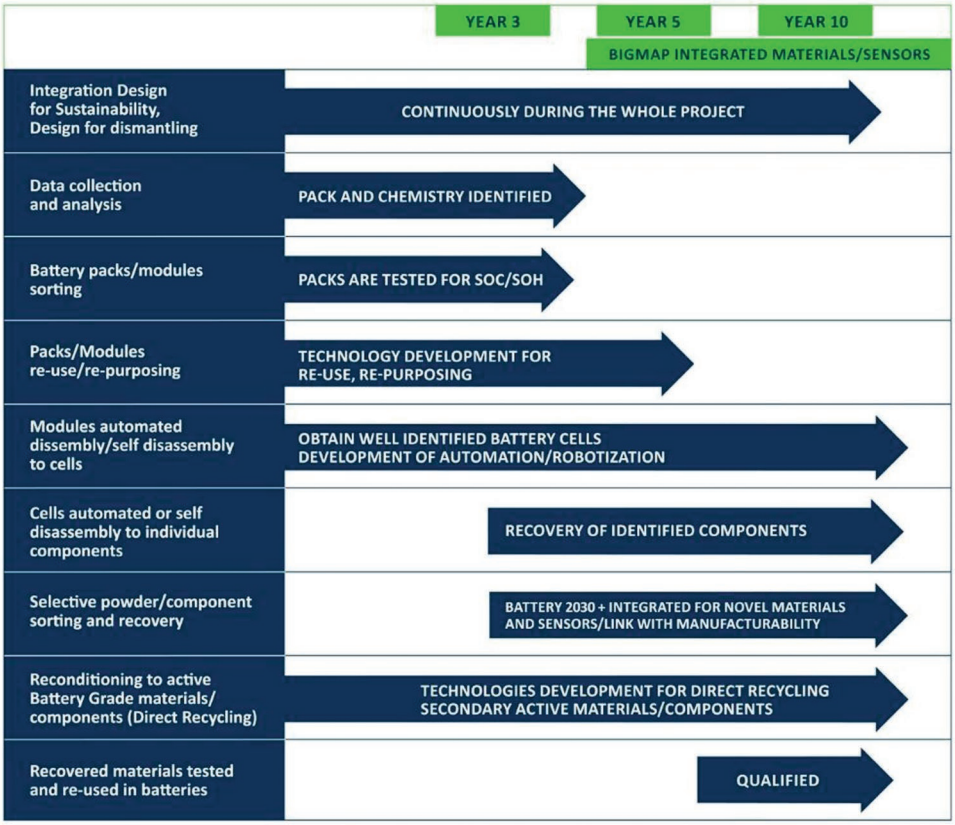

Figure 15. The ten-year roadmap for recyclability within BATTERY 2030+.

addressed. The first theme pertains to the accelerated discovery of battery materials via a fundamentally improved understanding of their functional interfaces. Within the field of material research, we think Europe can play a leading role by the development of material acceleration platforms (MAP) with specific focus on designing and improving key battery components. The second theme deals with the integration of smart functionalities into batteries that will increase safety, reliability, and cycle life. Here, the development of self-healing mechanisms holds significant promise to enhance battery life-time. Finally, we believe that blue-sky research shaping new technology must consider the manufacturability aspects of batteries and, facing the challenges of a climate-neutral society, the recyclability of batteries. In conclusion, over a time frame of ten years, we will develop a circular model incorporating specific R&I actions, based on the considerations developed in the roadmap detailed above.

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Conflict of Interest

The authors declare no conflict of interest.

Keywords

battery 2030+ roadmap, battery interface genome, chemistry neutral approach, manufacturing, materials acceleration platform, recycling, smart battery functionalities

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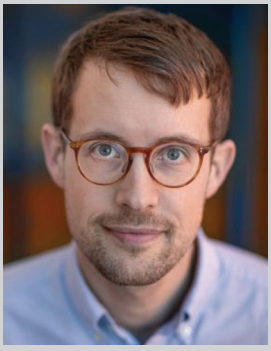

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Kersti Hermansson is professor of Inorganic Chemistry at Uppsala University. The group conducts research on multi-scale modelling techniques, especially at the electronic and atomistic levels. Redox chemistry of nano-structured metal oxides, aqueous solutions, liquid/solid interfaces, and computational vibrational spectroscopies are special interests. She is a founding member of the European Materials Modelling Council and member of its Board of Directors, and a WP leader of the European BIG-MAP project (The Battery Interface Genome—Materials Acceleration Platform). She is a fellow of the Royal Swedish Academy of Sciences (KVA).

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Saibal Jana received his Ph.D. in Chemistry from the Indian Institute of Technology (IIT) Kharagpur, India. After his Ph.D., he worked as a postdoctoral research associate in JNCASR, India; Brain-Korea Postdoctoral Fellow at Hanyang University, South Korea; and postdoctoral research associate at the University of Liverpool. Dr. Jana is currently working as a postdoctoral fellow at Karlsruhe Institute of Technology, Germany. His research interests include reaction mechanism, catalysis, TADF, and the design of novel anode materials for rechargeable battery technology. Currently, his research is focused mainly on solid electrolyte interphase (SEI) formation study.

Lara Jabbour holds a Ph.D. in Materials Science from Université Grenoble Alpes (France, 2012). During the last eleven years, she worked as a researcher and project manager in the public and private sector, in France and in the UK, on the formulation, processing and characterization of composite and polymers materials for various applications: energy storage/conversion, industrial and aerospace. Moreover, she specialized in innovation management, technology transfer, and European/Institutional funding project management. In 2017, she joined The French Alternative Energies and Atomic Energy Commission (CEA) and she is currently Program Manager for the structural, organic, and printed electronics division.

Josef Kallo earned his Ph.D. at General Motors and the University of Ulm in 2004. As a project engineer at GM he worked on electrochemical system modelling and vehicle system tests. Later, at the German Aerospace Center Stuttgart, he performed battery and fuel cell system research for mobile, stationery and aircraft applications. As institute director for Energy Conversion and Storage at the University of Ulm he achieved the complete integration of a fuel cell/battery propulsion system for aircraft applications. He is CEO of H2FLY, a multimillion equipped start-up with 50 engineers to commercialize fuel cell battery propulsion in aircraft applications.

Arnulf Latz is professor for electrochemical multiphysics modeling at the University of Ulm, the head for Computational Electrochemistry at the German Aerospace Center (DLR), and in the board of directors at the HIU Ulm for Electrochemical Energy storage. He spent 10 years in USA and Germany, over 10 years at the Fraunhofer Institute for Industrial mathematics, and since 2008 he is developing advanced continuum models and simulation tools for studying transport and reaction processes in electrochemical storage devices. He developed the battery simulation tool BEST. His research interests are modeling aging and degradation processes in Li-ion batteries, Li-conversion batteries, and Post Li-ion batteries developing advanced transport theories for electrolytes. He is author of 250 research papers.

Henning Lorrmann, diploma engineer for nanostructure sciences and head of the Fraunhofer R&D Center Electromobility in Bavaria, over 12 years professional experience in the application and management contract research projects in the field of electrochemical energy storage. Involved in >20 national and EU collaborative projects on battery development. Member of the BATTERY 2030+ group, expert and co-author and co-chair in the ETIP Batteries Europe, member of the steering committee and responsible for the thematic field “recycling” in the Fraunhofer Battery Alliance and representative of the Fraunhofer-Gesellschaft and member of the Association Delegation in the Batteries European Partnership Association BEPA.

Ole Martin Løvvik is chief scientist at SINTEF Sustainable Energy Technology and professor at the University of Oslo. His background is within computational materials science, with a focus on atomic-scale simulations on materials for sustainable energy applications. This includes hydrogen separation membranes, hydrogen storage materials, thermoelectric generators, solar cell materials, as well as battery materials.

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Marcel Meeus has a Ph.D. in Chemistry from the Catholic University of Leuven, Belgium. He completed a professional career at the company Umicore in various functions but with a strong focus on the development, production and marketing of primary and rechargeable battery materials. After retirement he is managing director of a consulting company Sustesco BV mainly oriented to energy, batteries, and the hydrogen economy. As such he acts as technical consultant to EMIRI.

Elie Paillard is associate professor at Politecnico di Milano in Italy. Has been working on polymer and ionic liquid electrolytes for lithium batteries since 2004 (Ph.D. at LEPMI, France and post-doc at NC State University, USA). From 2010 in Germany, he added few Li-metal and Li-ion topics (nanostructured conversion/alloying anodes, binders, Li-O_2, post-mortem, additives, etc.) at MEET and the Helmholtz Institutes in of Ulm and Muenster. He currently focuses on Li, Na, Li, Ca-ion/metal interfaces and electrolytes. He co-authored 72 scientific articles, 10 patents, and 3 book chapters.

Simon Perraud holds a Master of Science from ESPCI Paris (2004), a Ph.D. in Physics from the Université Pierre et Marie Curie (2007), and a Habilitation degree from the Université Grenoble Alpes (2013). From 2004 to 2007, he was a doctoral researcher at the Nippon Telegraph and Telephone Corporation (Japan), investigating electronic properties of semiconductor heterostructures. He earned the Award of the Japan Society of Applied Physics in 2008. Simon joined CEA (France) in 2008. He is the deputy director at CEA Liten, with about 1000 staff focused on the development of innovative technologies for the energy transition.

Tobias Placke is head of the division "Materials" at the MEET Battery Research Center, of the University of Münster in Germany. Dr. Placke's present research is devoted to the tailor-made synthesis and characterization and understanding of advanced negative and positive electrode active materials as well as inactive components for high-energy lithiumion batteries. He focuses on the development of alternative sustainable battery storage technologies such as dual-ion batteries. Dr. Placke has 10 years of experience in the field of material science and electrochemistry, and he is (co-)author of more than 100 scientific publications and detains 6 patents.

Christian Punckt is the Managing Director of the German Cluster of Excellence POLiS (Post-Lithium Storage). After his Ph.D. in Physical Chemistry in Berlin, he went to Princeton University in 2007, where he studied electrochemical applications of graphene-based materials, graphene-based polymer composites, and graphene production. From 2011 until 2014, he worked at Vorbeck Materials Corp., a company for graphene-based conductive inks and materials for energy applications. In 2014, he started at Karlsruhe Institute of Technology with science management, focusing on nanomaterials- and energy storage-related projects. Christian is active in the Graphene Flagship and works as a standardization expert.

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Janna Ruhland is a chief engineer at the Institute of Production Science at the Karlsruhe Institute of Technology. In her group, methods and processes for the production of li-ion and post-lithium-ion batteries are investigated. To this end, new machines and processes are being developed for the flexible production of battery cells in terms of material, format, and number of units.

Edel Sheridan is a senior business developer at SINTEF, Norway. She is working with the battery research community and the networks: Batteries Europe ETIP, Battery 2030+ and European Energy Research Alliance for Energy Storage (EERA ES), etc. and developing key strategic documents. She is the technical leader of the Batteries Europe ETIP and a member of the executive board of the Battery European Partnership Association (BEPA). Her research focuses on materials development for supercapacitors, Li ion, Mg ion, and Zinc-air batteries and worked on membranes and sensors. Edel holds a Ph.D. in electrochemistry from the National University of Ireland, Maynooth.

Helge Stein is a tenure track professor at the Karlsruhe Institute of Technology, teaches at the Institute of Physical Chemistry and researches at the Helmholtz Institute Ulm. His research interests are the accelerated discovery, understanding and upscaling of energy conversion and storage materials by the integration of combinatorial synthesis, and high-throughput characterization with machine learning and data management. He builds a platform for accelerated electrochemical energy storage research (PLACES/R). Through controlled variation and centralized data ingestion of composition, structure, morphology, and processing he seeks to understand why some energy storage materials work and how unwanted processes like degradation can be mitigated.

Jean-Marie Tarascon is professor at the College de France holding the chair "Chemistry of solids—Energy," but much of his early career was spent in USA where he discovered the plastic Li-ion technology. Back to France in 1995, he created the European network of excellence ALISTORE-ERI and more recently the French network on electrochemical energy storage (RS2E). Tarascon's present research is devoted to battery materials/electrolytes, novel reactivity concepts, chemistries beyond Li, and sensing. He is the author of approximately 700 scientific papers, detains approximately 100 patents, and received many honors, with the last ones being the 2020's Balzan prize.

Victor Trapp is head of Marketing and Sales at Fraunhofer ISC, Wurzburg, Germany. Early nineties, he started research on material technologies for fuel cells and PV and established a global team for upscaling and marketing carbon-based fuel cell components at SGL Carbon (1997). Later he was involved in business development for carbon materials for batteries and super-caps. In 2011, he established a battery materials department including research on solid state electrolytes at Fraunhofer ISC. He is active in European battery and materials stakeholder organizations and devoted to pushing green material technologies into various markets such a recycling, biomaterials, sustainable packaging.

Tejs Vegge heads the Section for Autonomous Materials Discovery at the Technical University of Denmark, working on the development of autonomous methodologies for accelerating materials discovery and innovation processes. Prof. Vegge is an elected member of the Academy of Technical Sciences (ATV) and the Danish Government's Commission on green transportation and has published more than 180 papers in the field of computational design of advanced battery materials and next-generation clean energy storage solutions. He serves as coordinator of the Battery Interface Genome–Materials Acceleration Platform (BIG-MAP) project and as member of the executive board of BATTERY 2030+.

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Wolfgang Wenzel leads the department for multiscale modelling and materials design at the Institute of Nanotechnology at Karlsruhe Institute of Technology. He obtained his Ph.D. in Physics in 1989 at Ohio State University before moving first to Dortmund University and then to Karlsruhe University. His research interests are the development and application of multi-scale simulation methods to nanoscale structure formation and function. Further the development of these methods, he is actively involved in the EU project BIG-MAP on batteries and the coordination of the joint lab for virtual materials design of the Helmholtz association.

Martin Winter has researched in the field of electrochemical energy storage and conver-sion for more than 30 years. His focuses on the development of new materials, components, and cell designs for lithium ion, lithium-metal batteries, and alternative battery systems. He currently holds a professorship for "Materials Science, Energy and Electrochemistry" at the Institute of Physical Chemistry, University of Münster, Germany. He is founder and scientific director of MEET Battery Research Center at the University of Münster and of Helmholtz-Institute Münster (HI MS) "Ionics in Energy Storage," a division of Forschungszentrum Jülich. Martin Winter has received numerous awards and recognition's.

Andreas Wolf is a Master of Science in Functional Materials (Julius Maximilian University Wuerzburg). He has spent time at the University of New Mexico (2016–2017), internships at the BMW Group (2018–2019, department for adhesives) and in IFE Norway (2020, silicon anodes). He is research assistant at the Fraunhofer Institute for Silicate Research in the field of lithium-ion batteries. His Ph.D. focuses on interactive magnetic supraparticles in dynamic fluidic environments and their application as smart sensors in water purification and battery recycling processes. A key is the use of magnetic particle spectroscopy for live-analysis of magnetic nanoparticle relaxation phenomena.

Kristina Edström is professor of Inorganic Chemistry at Uppsala University Sweden and coordinator of the large-scale European research initiative BATTERY 2030+. She studies Li-ion batteries, Na-ion batteries, solid-state batteries, and other new sustainable battery chemistries. She studies interfaces between materials and components and she develops in situ/operando techniques. She leads the Ångström Advanced Battery Centre and the Swedish Battery Center BASE. She has more than 300 scientific papers. She is member of the Royal Academy of Engineering Sciences (IVA) and the Royal Academy of Sciences, honorary doctor at NTNU, Norway, gold medal from IVA, and she is a Wallenberg Scholar.