INVENTING THE BATTERIES OF THE FUTURE
Research Needs and Future Actions

BATTERY 2030+ ROADMAP
SECOND DRAFT
GLOSSARY

AI  Artificial Intelligence
AIMD  Ab Initio Molecular Dynamics
BIG  Battery Interface Genome
BIG-MAP  Battery Interface Genome – Materials Acceleration Platform
BMS  Battery Management System
BSH  Battery Self-Healing
CEI  Cathode Electrolyte Interface
CNT  Carbon Nanotube
CSA  Coordination and Support Action
DoE  Department of Energy, US
EBA  European Battery Alliance
EMMC  European Materials Modeling Council
Energy density  Energy per unit volume (Wh/l)
EPR  Extended Producer Responsibility
EPR  Electron Paramagnetic Resonance
FBG  Fiber Bragg Grating
FOEWS  Fiber Optic Evanescent Wave Spectroscopy
HPC  High Performance Computing
HTS  High-Throughput Screening
KMC  Kinetic Monte carlo
KPI  Key Performance Indicator
LEAPS  League of European Accelerator-based Photon Sources
LENS  League of Advanced Neutron Sources
LFP  Lithium iron phosphate
LIB  Lithium ion Battery
LM  Liquid Metal
LMO  Lithium Manganese Oxide
MAP  Material Acceleration Platform
ML  Machine Learning
MOF  Micro Structural Optical Fibers
NCA  Lithium nickel cobalt aluminium oxide
NMC  Lithium nickel manganese cobalt oxide – LiNi1/3Mn1/3Co1/3O2
NMC 532  Lithium nickel manganese cobalt oxide – LiNi0.5Mn0.3Co0.2O2
NMC 622  Lithium nickel manganese cobalt oxide – LiNi0.6Mn0.2Co0.2O2
NMR  Nuclear Magnetic Resonance
NPS  Nano-Plasmonic Sensing
PCF  Photonic Crystal Fiber
QRL  Quality, Reliability and Lifetime
RE  Reference Electrode
SEI  Solid Electrolyte Interphase
SET-PLAN  Strategic Energy Technology Plan
SWCNT  Single-Walled Carbon Nanotubes
SoC  State of Charge
<table>
<thead>
<tr>
<th>Acronym</th>
<th>Description</th>
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<tbody>
<tr>
<td>SP</td>
<td>Sensor Plasmonics</td>
</tr>
<tr>
<td>Specific energy</td>
<td>Energy per unit mass (Wh/kg)</td>
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<tr>
<td>TEM</td>
<td>Transmission Electron Microscopy</td>
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<tr>
<td>TRL</td>
<td>Technical Readiness Level</td>
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<tr>
<td>TBMS</td>
<td>Thermal Battery Management System</td>
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<tr>
<td>XAS</td>
<td>X-ray Absorption Spectroscopy</td>
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<td>XRD</td>
<td>X-ray Diffraction</td>
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PREFACE

“Batteries are one of the key technologies to enable a carbon-neutral Europe by 2050”

The large-scale European research initiative BATTERY 2030+ – at the heart of a connected green society – presents the second draft of a roadmap expressing the long-term research actions necessary to enable the invention of the batteries of the future. This will ensure European leadership in this field, and contribute to the goal of a European fossil-free society by 2050.

BATTERY 2030+ is currently supported with a Horizon 2020 Coordination and Support Action (CSA) from 1st of March 2019 to 30th of May 2020. During this period, a roadmap identifying long-term research needs, as well as propositions for research and innovation actions to meet these needs, are formulated. A full version of the roadmap will be submitted to the European Commission at the end of February 2020.

The first draft of the roadmap was published at the end of July 2019. More than 1,200 stakeholders from academia, research organizations, industry, and public sector, who at that time had endorsed the initiative, have been given the chance to respond to the first draft, both through a written consultation and at different workshops organized all around Europe. We have visited most of the EU Member States and some of the associated countries to present and discuss our ideas. The second draft of the roadmap, disclosed in the present report, takes into account the inputs received during the written consultation and the workshops.

The vision of BATTERY 2030+ is to invent the batteries of the future, bringing together the smartest brains in Europe to join forces in speeding up scientific discoveries, creating synergies and avoiding over-redundant research. BATTERY 2030+ has a long-term focus, which is absolutely necessary to address the obstacles preventing current and future battery technologies from performing close to their theoretical limits, while at the same time minimizing environmental impact and cutting down lifecycle carbon footprint. BATTERY 2030+ will follow a “chemistry neutral” approach to explore a wide range of battery chemistries and technologies. This will provide breakthrough technologies to the European battery industry across the full value chain, enabling European leadership in both existing markets (road transport, stationary energy storage, etc.) and future emerging applications (robotics, aerospace, medical devices, internet of things, etc.). With this large-scale European effort, BATTERY 2030+ will also attract new and young talents, which is vital for long-term competence building in this field.

BATTERY 2030+ is thus initiating a strong battery research movement to create open discussions about the fundamental research needs for Europe. We are looking forward to your reactions on the content of this report. Use our webpage http://battery2030.eu to learn more, and endorse the BATTERY 2030+ initiative to join the community that will shape the next versions of the roadmap.

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1. Summary

“BATTERY 2030+ - at the heart of a connected green society”

We are just at the beginning of a battle against carbon dioxide emissions from the transport, power and industry sectors. A key component in this battle is the ultra-high performance battery, which will also play a major role for the ongoing digital transformation of our societies.

BATTERY 2030+ is the large-scale and long-term European research initiative addressing the challenges we face to invent the batteries of the future. It will give new concepts to support the development of a European battery industrial value chain, from raw materials to advanced materials, cells, packs, and end-of-life management, and to companies using batteries in different application – European batteries fit for purpose.

BATTERY 2030+ suggests long-term research directions based on a “chemistry neutral approach”. The research actions should enable several different kinds of battery chemistries, existing or future, to reach their full potentials by closing the gap between their respective practical capacity and theoretical limit. The ideas that BATTERY 2030+ propose will allow Europe to reach and overcome the ambitious battery performance targets agreed upon in the Strategic Energy Technology Plan (SET-plan) proposed by the European Commission. In addition, the BATTERY 2030+ long-term roadmap perfectly complements the short- to medium-term research and innovation efforts within Batteries Europe – the European Technology and Innovation Platform (ETIP).

The overall goal is to reach sustainable batteries with ultrahigh performance and smart functionalities fit for each application. With ultrahigh performance we mean energy and power densities approaching the theoretical limits, outstanding lifetime and reliability, enhanced safety and environmental sustainability and scalability to enable large-scale production of batteries at a competitive cost.

A first important challenge is to reach the highest battery performances. The discovery of new materials and new battery concepts must be accelerated. These new materials need to be stable in a battery context towards non-wanted corrosion or chemical side reactions. Special attention need to be paid to the complex reactions taking place at battery interfaces. These interfaces exist between electrode materials and the electrolyte, between electrodes and current collector, between the different materials components within an electrode, etc.

BATTERY 2030+ advocates the development of a Battery Interface Genome (BIG) – Materials Acceleration Platform (MAP) initiative, in which artificial intelligence (AI) will be utilized to drastically reduce the battery materials development cycle time. A central aspect will be the development of a shared European data infrastructure capable of performing autonomous acquisition, handling and utilization of data from all domains of the battery development cycle. Novel AI-based tools and physical models will be developed to utilize the large amounts of data, with a strong emphasis on battery materials, interfaces and interphases. The data will be 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.

The European research infrastructure landscape is well equipped to carry the ideas proposed in 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 Modeling Council. In addition, there are a number of synchrotrons and neutron facilities in Europe represented by the organizations LEAPS and LENS, respectively that are resources with potential to enable the BIG-MAP initiative.

A second important challenge is to enhance the lifetime and the safety of battery cells and systems. Both properties have a critical impact on the size, cost, and acceptance of future batteries. To reach these goals, BATTERY 2030+ suggests two different and complementary schemes: development of sensors probing chemical and electrochemical reactions directly at battery cell level and enhancing performance of batteries by using self-healing functionalities within battery cells.

New types of embedded sensors would allow for continuous monitoring of the “state of health” and “state of safety” of the battery. There are several different possible sensor technologies and approaches, including optical fibers, plasmonics, acoustics, electrochemical sensors, etc. As this will increase the complexity of the system, also manufacturability and recyclability must be taken into account to ensure affordable and scalable batteries of the future.

Self-healing means introducing passive and active components or molecules in different parts of battery cells, which can be released by external stimulus or can react continuously to prevent degradation of both the bulk electrode materials and the interfaces within the battery. Here, inspiration can be found in the area of drug delivery. In a 10 year perspective, a family of possible self-healing concepts will be available which are targeted for different battery chemistries dependent on where the batteries are to be used. Sensors will be available that can be seamlessly integrated at cell level and which can control thermal runaway reactions, ageing phenomena and release self-healing agents to provide batteries with several times longer life than today. The development of new sensors with high sensitivity and accuracy and at a low cost offer the possibility to access a full operational smart battery. The integration of these new technologies at the pack level with an efficient BMS with a real active connection to the self-healing functions is one objective of the roadmap for BATTERY 2030+.

Manufacturability and recyclability of battery materials, cells and systems are cross cutting areas that will be integrated in all research areas identified in the roadmap. This will enable the project to take into account the specific needs and boundaries of a circular economy already in an early stage of development.

Within 10 years of BATTERY 2030+ research efforts the impact on battery technology (compared to the current state of art) will be the following:

- reducing the gap, by at least a factor of two, between accessible and theoretical battery performances (energy density and power density);
- improving, by at least a factor of three, the battery durability and reliability;
- cutting down, by at least a factor of five, the life-cycle carbon footprint of batteries (for a given electricity mix);
- reaching a battery recycling rate of at least 75%, and a critical raw material recycling rate close to 100%.

BATTERY 2030+ has the ambition to drive a 10-year large-scale European effort for transformational research in the field of batteries, which will be unique in an International context. BATTERY 2030+ will continue to propose new research and innovation areas to overcome the main roadblocks to achieve ultrahigh performance batteries that are safe, affordable, and sustainable with a long lifetime. With this approach BATTERY 2030+ can be one tool to achieve the European mission of a fossil-free society by 2050 (see Figure 1).
2. Introduction

“The development of lithium-ion batteries, awarded with the Nobel Prize in chemistry 2019, is just the first step – much more is to be discovered and utilized”

What will the European energy system and transport sector look like 25 to 30 years from now? How can batteries, as one key technology support Europe to live up to the UN sustainability goals, such as affordable and clean energy, climate action, industry, innovation, infrastructure and new jobs preventing poverty? Everything points to an era where electrification will be one of the main drivers for a carbon neutral society. In this context, batteries will be a key technology, enabling energy storage with a very high round-trip efficiency. To really make a difference, Europe needs new generations of ultrahigh-performance, reliable, safe, sustainable and affordable batteries.

In the report High-energy batteries from 2030+ published in 2017 by Fraunhofer ISI [1], it is stated that “there will be a drastic increase in the global demand for batteries in the next decade if electric vehicles, portable digital devices and stationary decentralized energy storage applications continue to take off”. It is also suggested that Europe alone would need a yearly cell production capacity of at least 200 GWh up to the TWh range, to ensure access to batteries for European companies. All international institutes making estimates of the future lithium-based battery market forecast a rapid growth in the next ten years. In this context, the European Union is strongly supporting the establishment of a competitive battery value chain in Europe, as explained in the report published in April 2019 [2] by the European Commission. This document is to provide a state of play of the main actions needed to be undertaken within the framework of the Strategic Action Plan on Batteries which was published in March 2018 [3]. A strong research and development community for batteries is vital for Europe’s future competitiveness.

Even if the current generation of lithium-ion batteries will be the dominating form of high-capacity rechargeable batteries in the nearest future, there is a need for next-generation sustainable and affordable batteries, fit for purpose, that have higher energy and/or power content, longer lifetime, more predictable state of health and a wider temperature operation range. Preferably, all these parameters should be fulfilled in the same battery cell simultaneously, and it must meet high safety standards. This is a highly challenging task. Disruptive ideas are required that can enable the creation of the batteries of the future. In particular, there is an urgent need to develop novel tools and processes that can accelerate the discovery of new battery materials with improved stability at interfaces, to add smart functionalities into battery cells, and to support new manufacturing methods and efficient recycling measures. BATTERY 2030+, as a long-term and large-scale research initiative, aims to leapfrog the battery research field, and support Europe to coordinate the battery research community in the different member states to collaborate on unified goals, and to reduce the risk for fragmentation or over-redundancy in battery research. The BATTERY 2030+ roadmap will suggest a number of critical actions to take within the next 10 years, to
provide breakthrough technologies to the European battery industry across the full value chain, enabling long-term European leadership in both existing markets (road transport, stationary energy storage) and future emerging applications (robotics, aerospace, medical devices, internet of things, etc.).

Battery development is at a crossroad. The rechargeable battery market is already significant, and expected to experience a very fast growth in the coming years. At the same time, the future is open for radically new ideas and concepts, in the way we discover novel materials, engineer interfaces, and design batteries with added-value smart functionalities.

BATTERY 2030+ focuses on transformational research at low technological readiness levels (TRL, typically between 1 and 3), that will transfer new knowledge and concepts across all high TRL levels. The BATTERY 2030+ long-term roadmap perfectly complements the short- to medium-term research and innovation roadmaps established in the SET-Plan[2] and being developed by Batteries Europe[4] as well as the short-term industrial initiatives supported by the European Battery Alliance (EBA)[5] (see Figure 2). As an essential part of the European battery innovation ecosystem, BATTERY 2030+ will provide Europe with a competitive edge in the global race for clean energy technologies.

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**FIGURE 2.** The European Battery research and innovation ecosystem – the complementarity between the European Battery Alliance, Batteries Europe and BATTERY 2030+. BATTERY 2030+ will transfer new knowledge and technologies across the full value chain and across all TRL-levels.

This document presents the second version of the BATTERY 2030+ long-term research roadmap. It describes the most important opportunities and obstacles to address in order to develop ultrahigh performing batteries with higher energy and/or power content, longer life preventing ageing phenomena, which will be safe, sustainable and possible to manufacture and recycle with a low carbon footprint.
3. BATTERY 2030+, a chemistry-neutral approach with impact on future battery technologies

“BATTERY 2030+ aims for a visionary approach to invent the batteries of the future, contributing to solve environmental challenges.”

BATTERY 2030+ will take on a chemistry neutral approach to address the most important challenges that prevent the development of ultrahigh performance batteries. This means that the tools and processes suggested in this roadmap can be potentially used on any battery chemistry, including current Li-ion chemistries as well as on still unknown chemistries, creating an impact on both state-of-the-art and future electrochemical storage systems. Sustainable batteries of the future will be developed with tailor made performance and properties (e.g., high energy density, high power density, long cycle lifetime). In this section we first describe the current status of the field followed by the targets proposed by BATTERY 2030+, as well as the relation to other global roadmaps.

3.1.1. Current status

Several different types of rechargeable batteries are on the market, dominated by lead acid and Li-ion batteries. There is also a strong effort to development redox flow batteries.

The first commercial Li-ion battery was built and sold by Sony in the early 1990s. Since its market introduction, the Li-ion battery has increased its energy density by a factor of three while the cost has dropped by a factor of 15. Relying on this battery concept, a plenitude of efforts is underway worldwide to further increase battery performance by developing better storage materials, better electrolytes and more efficient new cell concepts.

While Li-ion batteries are used in applications ranging from electronic devices to electric vehicle applications just as well as in large scale storage regulating among other things grid quality, redox flow batteries are mainly targeting large scale storage applications. It has technical advantages, such as potentially separable liquid tanks and nearly unlimited longevity. It also has technical disadvantages such as low energy density and low discharge/charge rates.

As a consequence of the great progress in the field, electrochemical energy storage in batteries is regarded as a critical component in the future energy economy, in the automotive and in the electronic industry. While the technical demands in these sectors have been quite challenging, the need to replace fossil energy by energy from renewable resources is getting increasingly urgent. For 2030 and beyond, a global annual market of more than 1.8 TWh of batteries is foreseen.[6]

The current technological status in the field is summarized in Figure 3, where the capacities of the major rechargeable battery types are depicted. It should be noted that we are now entering a phase where the increase in performances is leveling-off, hence new solutions and ideas are sorely needed. By the current state of knowledge, it will be difficult or even impossible to
satisfy the future requirements in electrochemical energy storage with solutions that are based on these current technologies.

More details of the state of the art can be found in numerous text books [7][8][9][10].

![Figure 3. Current status of the most common rechargeable batteries.](image)

### 3.1.2. BATTERY 2030+ targets

The BATTERY 2030+ roadmap identifies both the obstacles to overcome and the tools to develop in order to reach ultra-high performance, reliable, safe, sustainable and affordable batteries. With its “chemistry neutral approach” BATTERY 2030+ aims at developing a generic toolbox and efficient processes for inventing the green batteries of the future, tailor made for each application. The research areas proposed in the BATTERY 2030+ roadmap can potentially be applied to any battery chemistry, creating an impact on both state-of-the-art and future electrochemical storage systems. This means that BATTERY 2030+ must lead to disruptive leaps in battery performance compared to the targets formulated in the SET-Plan Action 7. The generic approaches developed by BATTERY 2030+ will therefore boost performances, reliability, safety and sustainability in current and future lithium-ion and lithium metal battery chemistries, but also in post-lithium battery chemistries (sodium-ion, multivalent metal-ion, metal-air, etc.) as well as in future battery chemistries. Figure 3 shows how the SET-Plan depicts the different generations of batteries that should be the European targets the coming years. BATTERY 2030+ will be one strong enabler of the expected developments but also push the development to its limits.
FIGURE 4. The BATTERY 2030+ chemistry-neutral approach will have an impact on both state-of-the-art and future electrochemical storage systems.

BATTERY 2030+ aims to impact battery technology development (compared to the current state of art) by:

- reducing the gap, by at least a factor of two, between accessible and theoretical battery performances (energy density and power density) – see Table 1 where the practical and theoretical capacities for a number of rechargeable batteries are presented;
- improving, by at least a factor of three, the battery durability and reliability;
- cutting down, by at least a factor of five, the life-cycle carbon footprint of batteries (for a given electricity mix);
- reaching a battery recycling rate of at least 75%, and a critical raw material recycling rate close to 100%.

In addition to these highly ambitious targets, it should be noted that BATTERY 2030+ will also contribute to reach, at an accelerated pace, the key performance indicators identified in several battery technology roadmaps, including the SET-Plan[2] and Batteries Europe[4] at the European level. In an international perspective, we see the BATTERY 2030+ initiative as unique if it will be realized as a long-term effort, see below (3.1.3) where BATTERY 2030+ is compared to different international initiatives.
Figure 5 is showing theoretical data that are almost impossible to reach due to the need of including electronically additives, binders etc. in the electrodes of the cell. This will affect and dilute the theoretical capacity in practice. It is, however, clear that the “practical capacity” could come much closer to the theoretical ones than demonstrated today, both at battery cell level and even more so at battery pack level.

3.1.3. BATTERY 2030+ in an international context

How unique is BATTERY 2030+ in an international context? The international and European communities are aware of the strong needs to push the research front to reach ultra-high battery performances. In order to tackle these challenges, some of the larger countries have focused roadmaps formulating long-term efforts in battery research and development, comparable to the European SET-Plan. All of these roadmaps are, however, focused on specific chemistries and targets for reaching certain gravimetric and volumetric capacities at battery cell level. BATTERY 2030+ follows a completely different “chemistry neutral” approach, addressing disruptive concepts to make Europe a world-leader in future battery technologies.

In Appendix 1 we give a short presentation of the roadmaps from China, India, Japan, and US to give a broader perspective to the ambitions of BATTERY 2030+. Interesting to note is that both the Chinese and Japanese roadmaps have more ambitious capacity targets than the European SET-Plan (see Figure 24 in Appendix 1).
FIGURE 6. Joint perspectives of automotive battery R&D in China, Europe, Germany, Japan, and the USA [14].

In an overview, the general research strategies in the automotive sector of major global players are summarized in Figure 6.

In conclusion, a large-scale research initiative like BATTERY 2030+ is necessary for Europe to stay at the research front, to feed in new innovative knowledge and technology to the industrial level, and to support battery cell development, production, recycling and reuse in Europe.
4. BATTERY 2030+ research areas

“For Europe, battery production is a strategic imperative for clean energy transition and the competitiveness of its automotive sector. Moreover, the Commission's ‘new industrial policy strategy’ goal is to make the EU the world leader in innovation, digitisation and decarbonisation.” [5]

Battery research occurs across the full value chain of battery development. Battery research can be oriented towards battery cells, based on competences in chemistry, physics, materials science, modelling, characterisation, etc. It can also be oriented towards systems where the battery cells are integrated into packs, to be used in different applications. Here, the field relies on knowledge about electronics, electrical engineering, systems-control, modelling at system level, artificial intelligence (AI) and machine learning – just to mention some. Also, research in recycling has become more important and again rely on chemistry, metallurgy, physics and materials science linked to the use of new efficient characterisation tools.

The European research infrastructure landscape is well equipped to carry 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 Modeling Council. In addition, there are a number of synchrotrons and neutron facilities in Europe represented by the organizations LEAPS and LENS, respectively that 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 to integrate also other areas of research to enable cross fertilization.

The BATTERY 2030+ initiative currently includes four main research areas (materials acceleration platform, battery interface genome, sensing, self-healing), together with two cross-cutting areas (manufacturability and recyclability) which will be presented in the following chapters.

Chapter 4.1 describes a plan to accelerate the exploration and discovery of new battery materials, electrolytes and interfaces/interphases, by the development and implementation of a Materials Acceleration Platform (MAP). The MAP will enable autonomous closed-loop materials discovery and development through the use of AI to orchestrate data acquisition and analysis from multi-scale computer simulations, experiments and testing. This also includes the development of autonomous high throughput synthesis robotics and experiments also utilizing the Europe large-scale synchrotron and neutron facilities.

Chapter 4.2 focuses on interfaces in batteries which are arguably the least understood part of the battery, despite the fact that most of the critical battery reactions occurs there, e.g. the formation of dendrites, the solid electrolyte interphase (SEI) and the cathode interface (CEI). Accelerated design of battery materials requires a detailed understanding of the fundamental
“Battery Interface/Interphase Genome” (BIG), but to date interfaces/interphases have mainly been studied “post mortem” and with ex situ techniques. By combining the efforts in the MAP-part, where methods such as generative deep learning and multi-scale modelling will be combined with high throughput experiments as a part of BIG, new accelerated discoveries can be made. Experimentally this means studying and controlling interfaces and interphases in situ and operando as a battery cell is operating. This will enable us to take large steps towards better and more reliable batteries of the future[15].

By integrating the actions taken in Chapters 4.1 and 4.2, the aim is to establish predictive BIG models depicting the spatio-temporal evolution of interfaces and interphases which can be integrated into the MAP, leading to the “BIG-MAP”.

Chapters 4.3 and 4.4 are devoted to smart battery functionalities. The vision of BATTERY 2030+ is to inject smart sensing and self-healing functionalities into battery cells with the goal to increase the battery durability, enhance its lifetime by extending the reliable operation, lower its cost per kWh stored, and finally significantly reduce its environmental footprint. Non-invasive sensing technologies with spatial and time resolution will be developed to monitor battery cell key parameters when it is in operation and to determine defective spots or components within the cells that need to be repaired by injection/addition of self-healing functions. Sensing, being upstream of self-repair, will be presented next with its own goals for development, and then the suggested vision for self-healing will be described.

Chapter 5 describes two cross-cutting research areas. The new materials and interfaces/interphases designed using the BIG-MAP approach, as well as the novel sensing and self-healing functionalities integrated within battery cells, must be able to be up-scaled, manufactured and recycled simply and affordably. Chapter 6.1 describes the steps to ensure manufacturability and likewise Chapter 6.2 describes the steps to ensure recyclability. Chapter 6 discusses the need to enlarge this large-scale research initiative with new areas of studies, which should be ambitious and in line with the “chemistry-neutral” approach followed by BATTERY 2030+.

These different research areas will benefit from strong synergies between each other. The most obvious interactions are summarized in figure 7:

- sensors integrated down the battery cell level will provide a huge amount of data for the research community, which will be exploited in a systematic way by feeding the artificial intelligence used in the materials acceleration platform;
- sensing and self-healing functionalities will be strongly connected via the battery management system (BMS), which will trigger self-healing based on the information coming from the sensors;
- the materials acceleration platform and the battery interface genome will be powerful tools to discover new materials and engineer battery interfaces, and in particular will be used to discover or optimize self-healing materials and chemicals;
finally, the development performed in the cross-cutting research areas (manufacturability, recyclability) will ensure that it will be possible to manufacture and recycle in a efficiency way the next-generation battery cells integrating new materials and engineered interfaces, sensors and self-healing functionalities.

**FIGURE 7.** The link between the different research areas described below.

### 4.1. Materials Acceleration Platform (MAP)

Materials discovery and development is a fundamental need that crosscuts the entire clean energy technology portfolio, ranging from energy generation 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 10 years from initial discovery to commercialization. In BATTERY 2030+ we outline a radically new path for accelerated development of ultra-high performance, sustainable and smart batteries, which hinges on the development of faster and more energy- and cost-effective methods for battery discovery and manufacturing.

In this Chapter, we outline the opportunities, challenges and perspectives of establishing a community wide European battery “Materials Acceleration Platform” or “MAP”, which will be integrated with the Battery Interface Genome (BIG) described below. The proposed BIG-MAP infrastructure is modular and highly versatile, in order to be able to accommodate all emerging battery chemistries, materials compositions, structures and interfaces. Following the format of the Mission Innovation Clean Energy Materials (Innovation Challenge 6) MAP
Roadmap[16], a MAP utilizes Artificial Intelligence (AI) to integrate and orchestrate data acquisition and utilization from a number of complementary approaches and technologies, which are discussed in the sections below.

![Diagram of MAP components](image)

**FIGURE 8.** Key components in establishing a battery MAP.

Realization of 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 inverse design and tailoring of materials, processes and devices. Ultimately, coupling all elements of the MAP will enable AI-orchestrated and fully autonomous discovery of battery materials and cells with unprecedented breakthroughs in development speed and performance.

Successful integration of computational materials design, AI, modular and autonomous synthesis robotics and advanced characterization will lay the foundation for accelerating the traditional materials discovery process dramatically. The creation of “self-driving” laboratories capable of designing and synthesizing novel battery materials, and to orchestrate and interpret experiments on-the-fly will create an efficient closed-loop materials discovery
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process. Its implementation constitutes a quantum leap forward 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 relied extensively on an Edisonian (trial-and-error based) approach, where each step of the discovery value chain is sequentially dependent upon the successful completion of the previous step(s).

In recent years, a number of examples have emerged, where close integration of virtual (typically atomic-scale) computational materials design and operando characterization[17] techniques in a circular design loop can accelerate the discovery cycle for next-generation battery technologies, e.g. high-capacity Li-ion cathodes[18] and materials for secondary metal-air batteries[19], but further acceleration is needed to reach the highly ambitious goals of BATTERY 2030+. Ideally, such a circular materials development process will integrate experimental and theoretical research in a closely coupled development platform, which 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 the MAP.

Data-infrastructures and databases are central requirements for accelerated rational design of battery materials and interfaces, to ensure access and interoperability of high quality data from multiple sources, e.g. experiments, testing and modeling. A large number of ongoing efforts in Europe and beyond aim to create extensive, flexible and sharable data-bases and repositories[20], [21] for experimental data. Additionally, computational infrastructures like PRACE and EuroHPC, and platforms like UNICORE[22], [23], SimStack[24], AiiDA[25] and Materials Cloud[26] facilitate efficient and reliable high-throughput calculations. To fully exploit this data, extensive efforts from e.g. the European Materials Modelling Council (EMMC)[27] have been placed to develop ontologies (e.g. EMMO), i.e. a common knowledge-based representation system to ensure interoperability between multiple scales and different techniques and domains in the discovery process. A battery ontology 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 than 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[28]. The simulation of batteries require insight from very different length and time scales, i.e. following the guidelines of the EMMC: (1) Electronic scale, allowing the description of chemical reactions: electronic Density Functional Theory (DFT); Ab Initio Molecular Dynamics (AIMD). (2) Atomistic and mesoscopic scale: Molecular Dynamics (MD) and Kinetic Monte Carlo (KMC) simulations. (3) Macroscopic scales: continuum simulations. Presently, a single computational model for virtual materials design that encompasses all these phenomena is beyond the limits of current computing power and theory. To address this challenge, single-scale models must be
combined to multi-scale workflows, e.g. through deep learning models. Multi-scale modelling
techniques are currently being developed, for example, to optimize real and virtual electrode
microstructures[29], study the effects the fabrication process on cell performance[30], and
electrode surface film growth[31].

**Experimental characterization of materials and interfaces** at large-scale research facilities,
such as synchrotron and neutron scattering facilities, play a critical role in ensuring sufficient
acquisition of high-fidelity data describing battery materials and interfaces. 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 are discussed in detail in Chapter 4.3.

**Autonomous synthesis robotics**, which can be controlled and directed by a central AI, is a
central element in closed-loop materials discovery. Highly automated, high-throughput
syntheses are now becoming state-of-the-art for organic and pharmaceutical research[32],
[33], and examples are also emerging in the development of solids and thin-film
materials[34], [35]. For energy storage materials, robotic-assisted synthesis and automation
has opened the field to high-throughput screening of functional electrolytes and active
materials comprising anode and cathode. In combination with computational approaches
including, e.g., data-mining, correlation of structure-property relations and performance of
battery active materials, robotics has had a significant impact on the discovery of novel and
promising materials[32].

**Experimental and computational high-throughput screening** of large compound libraries
for activity in accelerated formulation of the relevant battery materials via the use of
automation, miniaturized assays, and large-scale data analysis can accelerate materials
discovery by up to one order of magnitude[36], [37]. A few examples of fully automated
high-throughput screening (HTS) system for electrolyte formulation, cell assembly and
selected relevant electrochemical measurements are now available[38], e.g. at the MEET
Battery Research Center in Germany.

**Artificial Intelligence in materials discovery** offers great prospects[15] but the complexity
and challenges for autonomous discovery of novel battery materials and interfaces are at a
much higher scale of complexity than present applications. The availability of vast, curated
data sets for training of the models is a prerequisite for the successful application of AI/ML-
based prediction techniques. Software packages like ChemOS[39] and Phoenix[40] have
been used in prototypical applications to demonstrate key components of an autonomous
(self-driving) laboratory, which has not yet been achieved for battery applications.

### 4.1.2. Challenges

**Availability of curated data**: The development of predictive models to design future
batteries requires thorough validation on the basis of curated data sets with diverse data
quality (fidelity). In particular, the validation of the complex models required for (inverse)
design[41] of battery materials and interfaces requires the integration of high fidelity data covering complementary aspects of the materials and device characteristics. Presently, such data sets are (too) sparse and cover only a fraction of the required data space.

In order to accelerate the development of future ultra-performing battery technologies, a consolidated strategy to overcome present bottlenecks must be implemented to ensure the success of the BATTERY 2030+ initiative. Presently, the exploitability of existing data and databases remains (very) low, in part because of the vast size of the design space, in part because system requirements impose constraints on materials that go beyond the optimization of individual performance indicators. A central aspect is uncertainty quantification and fidelity assessment of individual experimental and computational techniques, as well as in generative deep learning poses a key challenge. Here, the central aspect is “knowing when you don’t know” and knowing when additional data and training is needed. [42]

FIGURE 9. 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 acquisitioning data when the given method/data is most valuable (adapted from [42]).

While machine learning can potentially yield massive acceleration in the screening and identification of, e.g. structure-property relations of inorganic energy materials[43], a key challenge in the discovery of battery materials and interfaces is the development of
autonomous workflows for extraction of fundamental relations and knowledge from sparse datasets[44], spanning a multitude of experimental and computational time- and length scales.

**Challenges for closed-loop materials discovery:** In order to ensure full integration of data from experiments and tests into the MAP, automated protocols for data acquisition and analysis must be developed. Presently, there are only few examples of automated robotics for solid state synthesis[35] and more importantly, automated approaches for characterization of battery materials and cell are either lacking or dramatically underdeveloped. A number of machine learning based tools have recently been developed for a number of relevant characterization techniques, e.g. XRD and XAS[45], [46]. These tools will enable an automated analysis, but a wider portfolio of techniques with high-predictability is needed to support a fully autonomous materials discovery platform.

An important bottleneck towards closed-loop discovery is the lack of robust and predictive models for key aspects of the 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 under 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.[42]

**4.1.3. Advances needed to meet challenges**

**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, design of new liquid or solid electrolytes, and development beyond Li-ion battery chemistries, as well as new experimental and computational tools to understand complex redox reactions at the heart of these electrochemical systems, to name only few. World leading initiatives already exist at both the multinational level, e.g. Alistore-ERI, and the national level with for instance the French network on electrochemical energy storage and conversion devices (RS2E), the Faraday institution in England, the CELEST consortium in Germany, etc. demonstrating that partnerships can be created beyond individual laboratories. The European research community is ready to support a truly European research effort dedicated to advance 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 environment already existing.

**Autonomous synthesis robotics:** Until today, comprehensive electrochemical characterization of battery materials and testing on the cell level is one of the major bottlenecks for the development speed of new battery materials and interfaces. In order to explore larger classes of materials in the context of specific applications, it is essential to further the development high-throughput synthesis robotics that address both electrolyte formulations and electrode active materials, as well as the combinations thereof both for the characterization of the materials as such, but as well in the context of functional cells.
High throughput/high fidelity characterization: Even though, more and more approaches towards high-throughput testing of battery materials are reported in literature[47]–[49], many electrochemical tests do not work on short time scales, in particular cycling experiments can take days to months and years[50]. In order to exploit the opportunities generated by the vast number of samples, an automated high throughput infrastructure for 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 a filtration by identified lead candidates. The combination of physics-guided data-driven modelling and data generation is required in order to enable high-throughput testing of batteries and their incorporated active materials in the future, and thus to develop a batteries materials platform for accelerated discovery of new materials and interfaces.

A cross-sectorial data-infrastructure: Accelerated materials innovation relies on an appropriate and shared representation of both data and the physical and chemical insights obtained from it,[33], [51] posing a substantial challenge to the international research community to join forces in establishing, populating and maintaining a shared materials data infrastructure. Establishment of a common data-infrastructure will help to ensure interoperability and integration of experimental data and modelling in a closed-loop materials discovery process across institutions in real time. Realization of such an infrastructure will make the data generated by individual groups and consortia instantly available to the community at large and drastically shorten the R&D cycles. The MAP will pioneer such an infrastructure based on a decentralized access model, where 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 and link models at different scales in a efficient and robust way. The large gain in time and accessible size in models on larger scales generally entails a sacrifice in detail and resolution. Releasing the full potential of (inverse) multi-scale modelling to support new materials and device design requires radically new approaches to bridge scales beyond the state-of-the-art that can be achieved by isolated research communities in individual countries[52]. Machine learning techniques and other physics-guided data-driven models can be used to identify the most important parameters, features or fingerprints[53]. The 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, such as former and ongoing centers of excellence in HPC applications such as NOMAD and MaX.

AI exploitation: AI-based generative models[54], i.e. probabilistic models for the observed data for spatio-temporal evolution of battery materials and interfaces, can significantly contribute to the goals of the MAP, and developing hybrid physics and data-driven models will be an essential part of the MAP. Presently, 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 the latter are typically unaware and thus may violate
physical laws. The key to overcome this dilemma are the development of hybrid models, where the prediction space of AI based models is constrained by laws of physics or where AI is used to adapt physical models. These models must be trained on the large curated datasets from advanced multi-scale computational modelling, materials databases and literature[55], and from in-operando characterization. These data must span all aspects of battery materials from synthesis to cell level testing[56].

**Unification of protocols:** The MAP will offer a unique opportunity to leverage the size of this effort towards the standardization of data from the entire battery value chain, by exploiting semantic access protocols enabled by EMMC and EMMO, as well as private groups with the goals of connecting academia and industry, materials modelling and engineering[57]. 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 design of materials, battery cell manufacturing and their end-use in everyday life devices.

**Inverse design of battery materials and interfaces** is effectively inverting the traditional discovery process by allowing the desired performance goals to define the composition and structure of the battery materials and/or interfaces, which best fulfills these targets without a priori defining the starting materials. Interfaces 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

**The autonomous BIG-MAP:** The forward vision is to develop a versatile and chemistry neutral framework capable of achieving a 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 inverse design of ultra-high performance battery materials and interfaces/interphases, and be capable of integrating cross-cutting aspects like sensing (Chapter 4.3) and self-healing (Chapter 4.4), as well as manufacturability (Chapter 5.1) and recyclability (Chapter 5.2) directly into the discovery process.

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

**In short term:** Develop a shared and interoperable data infrastructure for battery materials and interfaces, spanning data from all domains of the battery discovery and development cycle; Automated workflows to identify and pass features/parameters between different time and length scales; Uncertainty-based hybrid data-driven and physical models of materials and interfaces.

**In medium term:** Implementation of the Battery Interface Genome in the MAP platform (BIG-MAP), capable of integrating computational modelling, autonomous synthesis robotics
and materials characterization; Demonstrate successful inverse design of battery materials; Direct integration of data from embedded sensors in the discovery and prediction process, e.g. to orchestrate proactive self-healing.

**In long term:** Full autonomy and chemistry neutrality in the BIG-MAP platform established and demonstrated; Integration of battery cell assembly and device-level testing; Inclusion of manufacturability and recyclability in the materials discovery process; Demonstrate 5-fold acceleration in the materials discovery cycle; Digital twin for ultra-high throughput testing on cell level implemented and validated.

### 4.2. Battery interface genome (BIG)

Past experience has shown that when developing new battery chemistries or introducing new functionalities into an existing battery technology, interfaces hold the key to exploit the full potential of the electrode materials and to develop ultra-high performance, sustainable and smart batteries. The European battery R&D landscape consists of a multitude of research institutions, laboratories and industries, many of which pursue complementary approaches to tackle this challenge at a local scale. We will bring together this expertise with cross-sectoral competences, industrial partners and end-users to establish the Battery Interface Genome (BIG) and accelerate the development of radically new battery technologies.

Current research methodology relies largely on incremental advances made at a local scale, which are not pertinent to tackle the ambitious challenges outlined in this Roadmap. The MAP will provide the infrastructural backbone to accelerate our findings, while BIG will develop the necessary understanding and models to predict and control the formation and dynamics of the crucial interfaces and interphases, which are limiting battery performance. Furthermore, as it remains open which will be the winning battery technologies for large scale and grid storage, for mobility, etc., BIG will be highly adaptive to different chemistries, materials and designs, starting from (beyond) state-of-the-art in Li-ion technology, where substantial data and insights are available for the training of the models, to emerging and radically new chemistries.

Batteries comprise not only an interface between the electrode and the electrolyte, but a number of other important interfaces, e.g. between the current collector and the electrode or between the active material and the additives such as conductive carbon and/or binder, etc. Realizing this, any globally leading approach trying to master and (inverse) design battery interfaces must combine the characterization of these interfaces in time as well as in space (spatio-temporal characterization) with physical and data-driven models integrating dynamic events at multiple scales, e.g. from the atomic scale to the micron scale. Therefore, BIG aims at establishing the fundamental “genomic” knowledge of battery interfaces and interphases through time, space and chemistries.
The “Battery Interface Genome” can be related to the concept of descriptors in catalyst design[58], where the binding energy of important reaction intermediates scales with that of the descriptor, and the identification and quantification of the descriptor value enables an accelerated and accurate prediction of the rate of the total reaction. Identifying the multitude of descriptors (or genes) coding for the spatio-temporal evolution of battery interfaces and interphases is a prerequisite for inverse design process, and simply cannot be established within existing methodologies. This requires the improvement of the capabilities of multi-scale modelling, artificial intelligence and systematic multi-technique characterization of battery interfaces, including operando characterization, to generate/collect comprehensive sets of high fidelity data that will feed a common AI-orchestrated data-infrastructure in the MAP.

4.2.1. Current status
Battery interfaces and interphases is where the energy storage in batteries is facilitated, but also where many degradation phenomena are initiated, have always been a combined blessing and a major limitation to the development of batteries. For instance, the growth of the so-called solid electrolyte interphase (SEI) on graphitic anodes is one of the most crucial property to ensure the cycling stability of the Li-ion battery. Thus, when mastered, interfacial reactivity helps to extend the thermodynamic and kinetic stability of organic electrolytes used in batteries while when it is not controlled, continuous parasitic reactions may occur, thus limiting the cycle life of the battery. Understanding, controlling and designing the function of interfaces and interphases is therefore key for the development of ultra-performing, smart and sustainable batteries.

In comparison to the bulk dimensions of the electrode and electrolyte (~µm), the interface (or interphase) is several orders of magnitude smaller (~nm) and interfacial reactions are easily masked by their surroundings. Experimental and computational techniques must therefore be highly surface sensitive with exceptionally high resolution to probe such buried interfaces. Nevertheless, the experimental characterization of battery interfaces has been a long lasting challenge. Indeed, very few, if any, techniques are currently capable to provide a full description of the 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 develop chemical and engineering approaches to control the dynamics of the interfaces upon cycling. The most prominent approach is the use of electrolyte additives, which react inside the cell during the 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 taught the need to use several additives working in synergy to provide an efficient SEI. Accelerated development of such an SEI would thus greatly benefit from high throughput techniques and the AI-assisted rationalization outlined here.

To provide valuable insights into the spatio-temporal evolution of interfaces and interphases, ensuring interoperability and the coupling of scales is necessary. Usually, the complexity of
electrochemical systems forces a simplification of the simulations such that they only qualitatively mimic the real situation in the battery. Therefore, even if the proper theory for performing the necessary statistical averages are derived, the obtained parameters/descriptors may considerably deviate from the parameters of the materials in their more complicated electrochemical environment. A coupling with physics-aware data-driven methods will 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 with data of real materials.

A complete and closed mathematical description of the whole reaction mechanism is enormously challenging, since coupled ionic and electronic transfer reactions in electrochemical relevant environment include usually coupled multistep reactions\cite{59}, \cite{60} Often, these multistep reactions are either tremendously simplified or reaction steps are modelled in ideal environments\cite{61}. In specific cases, it is possible to combine DFT methods with classical approaches to improve the description of surface reactions\cite{62}, but generic approaches remain limited and an efficient and systematic coupling is still lacking.

4.2.2. Challenges
Despite decades of research, the details of interfacial reactions in the complex electrochemical environments in batteries remain a conundrum, e.g. the composition and function of the SEI. The structural properties depend in a highly complex and elusive manner on the specific characteristics of the composition of the electrolyte and structures of the electrode materials, as well as the external conditions. The complexity of such interphases arises from multitude of reactions and processes spanning a wide range of time- and length scales that define their formation, structure and, ultimately, their functionality in the battery.

Intensive efforts have been devoted in the past years to uncover the complexity of the interface dynamics and to control its reactivity and functionality, generating enormous dataset which depth remains largely under exploited. Hence, a complete paradigm shift is needed in order to address this fundamental challenge. For that, data must be collected, handled and analysed in a more systematic and automated/autonomous manner, e.g. to be accessible to the central BIG-MAP AI orchestrating the accelerated discovery process. To ensure a meaningful synergy between experiments, simulations and AI-based models, the simulations and models should become more realistic and closer to experimental conditions. Similarly, the experimental conditions should be made as ideal as possible to decouple the different effects and reactions, especially for the initial training of the hybrid physics-aware models discussed previously.

In this regard, key challenges include the development of new multi-scale modelling concepts including physics-aware data-driven hybrid models to identify interphase descriptors, the development of new characterization techniques and standardization of experimental data and observables as inputs to physical models to make the link between observables and descriptors.
The fundamental understanding is the first step for controlling the complex and dynamic processes at the interfaces in emerging battery technologies and thus hold the key to developing ultra-high performance, sustainable and smart batteries, fully exploiting the potential of the electrode and electrolyte materials. 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. These should selectively provide information on the interface region, and special efforts must be paid at coupling complementary experimental, simulation-based and AI-based modelling tools[63]. It can be envisioned that mature battery interface/interphase characterization techniques can provide high-throughput experimental input on battery interfaces during operation. Today, the analysis of experimental results are however often too time consuming. One of the key challenges in establishing BIG is to automate the acquisition, curation and analysis of enormous datasets that will be generated. This data will feed the physics-aware data-driven hybrid models that will help to better understand and predict interface and interphase properties.

This will only be possible if data sets are created of reliable potential, time and spatially resolved experiments, including data recorded under working conditions (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 on curated community-wide datasets spanning multiple domains in the discovery process will enable establishing the battery interface genome and the identification of key descriptors/feature vectors, e.g. through representation learning[64][65], for interface/interphase development and dynamics that have the potential to lay the foundation for inverse design of battery interfaces/interphases[56], e.g. using region-based active learning algorithms[66].

Understanding and tracking different types of uncertainties in the experimental and simulation methods, as well as the machine learning framework for, e.g. generative deep learning models[67] is crucial for controlling and improving the fidelity in the predictive design of interfaces. Simultaneous utilization of data from multiple domains, including data from apparently failed experiments[68], can accelerate the development of generative models that enable accelerated discovery and inverse design of durable high-performance interfaces and interphases in future batteries.

4.2.3. Advances needed to meet challenges
The development of new computational and experimental techniques targeting increased spatial resolution, time domains and operando conditions is needed to generate new insights into the construction of ultra-performing battery systems. This development is challenging for both theory and experiment, and enhanced collaboration between the disciplines is necessary to unlock the next generation of battery technologies. Experimental input is needed to identify realistic input parameters for the development of new computational models, and modelling results need to be validated against experimental results. Likewise, the interpretation of
experimental results can be done with higher precision if theoretical models can be used in combination with the experiments.

In order to develop the battery interface genome, high quality/high fidelity data and insights are required which ask for the development of superior operando experimental techniques for establishing atomic level understanding on smaller scales and a variety of different time scales and dimensions. Moreover, on-the-fly acquisition and analysis should be targeted to provide an instantaneous input for the materials acceleration platform developed in MAP. Hence, BIG offers a unique opportunity to develop a common European platform, as well as common European battery standards for data acquisition and data transfer, that could serve as a standard worldwide.

In addition to the continuous improvement and development of new experimental techniques and methodologies, a radical new way of combining experimental, theoretical and data driven techniques will be necessary. Advanced physics-based hybrid models and simulation techniques have to be used for interpretation of cutting edge operando experiments. Efficient methods for using the large data sets to determine descriptors of multi-scale/multi-structure theories have to be developed. With these technical advancements, new insights follow, which will allow us to control the access to a fine tuning of batteries interface and thus develop the next generation of ultra-performing batteries.

Currently, there is no shared infrastructure or large-scale database of battery-oriented interfaces properties available which compares to, e.g., existing structure databases for organic and inorganic materials[69], [70]. The implementation of 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, to gain information about the 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 from the current single-technique paradigm. At the high-throughput level, characterisation techniques should be organised in a way to allow for investigation of a large number of samples by providing the necessary meta-data. This requires workflows that can generate and analyse large amount of data in an automated/autonomous manner which would represent a jump toward defining a new methodology of acquiring data about 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 the cells performances with their chemistry. For that purpose, a check list of good practices should be defined and becoming the project characterization quality label. BIG thus represents a unique opportunity to design a common European strategy in which cycling data for each new chemistry, successful or not, will feed a common data-infrastructure that will be broadly accessible, e.g. by a central-AI orchestrating the materials discovery. To meet challenges on standardization of experimental data and
observables as input to physical models, the implementation of feed-back processes may be contemplated as pivotal. This will be achieved by creating a European database of battery-oriented materials properties and a standardized classification of interfacial phenomena as well as by defining common observables for physical modelling which will be used to initiate paths and feed-back loops for multi-scale integration of data sets 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 performances of batteries, which will contribute to a better integration between 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[28]. Through the use of AI-based techniques linking BIG and MAP together, complex connections/features between scales that are unavailable to humans will be recognized and areas available to reliable predictions will thus be extended to new realms. However, modelling interphases is complex owing to the variety of the involved phenomena. Here, we envision the development of more accurate models that address more realistic interfaces, aging and degradation as well as complex design scenarios, requiring adequate mathematical frameworks to couple electronic, atomistic and mesoscopic models with continuum models. Merging advanced multi-scale modelling and data analytics will master the complex coupling of relevant length and timescales, which is so pertinent for batteries. The development of inverse modeling techniques which map the data back to model parameters will be thus pursued.

4.2.4. Forward vision
To accelerate the discovery and (inverse) design of battery interfaces and interphases, a fully autonomous materials acceleration platform (MAP) in which BIG, autonomous material synthesis and characterization and battery cell assembly will be integrated, must be developed. 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, where one effectively inverts this process by allowing the desired performance goals to define the composition and structure which best fulfills these targets without a priori defining the starting composition or structure of the interface. In order to develop and implement suitable models for inverse design of battery interfaces/interphases, it is necessary to incorporate the relevant physical understanding, and the model should be capable of performing an inverse mapping from the desired properties to the original composition of the materials and external parameters/conditions. The generative deep learning models described in Chapter 4.1 represent an efficient way to optimize the data flow and build the required bridges between different domains, helping to solve the biggest challenges of battery interphases (Figure 10).

This reliance on statistical correlations renders descriptors an ideal tool for data driven AI methods. A promising route is the full integration of data driven methods and physical theory based simulations, where e.g. inverse modelling on experimental data sets is used to
determine reliably the interface descriptors of the detailed spatio-temporal evolution. Based on these, forward simulations give insight in the expected spatially resolved time evolution of the system. With the outlined approaches, this (finite) number of parameters/features can be extracted from combining many different, simpler experiments using modern mathematical inverse modelling techniques and extracting a 4-dimensional spatio-temporal continuous field of physical variables can then be reduced to determining a finite set of parameters.

Doing so, rather than empirical development of battery chemistry and assembly, which has been the norm so far, we aim at developing an inverse design of battery driven by data input. This will be made sequentially to achieve within 10 years a fully autonomous and automated platform, integrating computational modelling, material synthesis and characterisation, battery cell assembly and device-level testing (BIG-MAP). Finally, we envision the battery discovery platform and the battery itself as fully autonomous, utilizing, e.g. the sensors developed in Chapter 4.3 to send signals that can be understood by the central BIG-MAP AI to predict the spatio-temporal evolution of the interface. If the model predicts a potential failure at the interface, this will launch the release of a self-healing additives, as developed in Chapter 4.4, to pre-emptively heal the interface and eventually increase the battery lifetime. Furthermore, the development of such inverse design strategy will also benefit the investigation of production (see Chapter 5.1) as well as recycling process (see Chapter 5.2).

**FIGURE 10.** Generative model for 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 genetic algorithms or reinforcement learning based exploration [56].
Full integration of the Battery Interface Genome into the battery Materials Acceleration Platform (BIG-MAP) will occur stepwise according to the following combined timeline for Chapters 4.1 and 4.2:

**In short term:** Establish community wide characterization/testing protocols and data standards for battery interfaces; Autonomous modules for on-the-fly analysis of characterization and testing data using AI and simulations; Interoperable high throughput and high fidelity interface characterization approaches developed.

**In medium term:** Develop predictive hybrid models for the spatio-temporal evolution of battery interfaces; Demonstrate successful inverse design of model battery interphases; Implementation of the Battery Interface Genome in the MAP platform (BIG-MAP), capable of integrating computational modelling, autonomous synthesis robotics and materials characterization.

**In long term:** Full autonomy and chemistry neutrality in the BIG-MAP platform established and demonstrated; Demonstrate a 5-fold improvement in the interface performance; Demonstrate transferability of the Battery Interface Genome to novel battery chemistries and interfaces.

4.3. Integration of smart functionalities – sensing

Our increasing dependence on batteries calls for an accurate monitoring of the battery functional status so as to increase their quality, reliability, and life (QRL). Over the last decades, numerous on-board electrochemical impedance devices (EIS) together with the developments of sophisticated battery management systems (BMS) have been made along these directions, but with limited success. Whatever battery technology considered, its performances is governed by the nature and dynamic of the interfaces within the battery cell that relies on temperature-driven reactions with unpredictable kinetics. Although monitoring temperature is essential for enhancing cycle life and the longevity of the battery, this is not directly measured today at the cell level for EV’s applications. To drastically enhance battery cell QRL, a 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 is needed, i.e. fundamental science.

To challenge the existing limitations, we propose a disruptive approach to inject smart embedded sensing technologies and functionalities into the battery cell, capable of performing spatial and time-resolved monitoring (Figure 11).
FIGURE 11. A future battery having an output analyzer (perhaps comprising of optical fibers to collect parameters such as temperature, pressure etc along with a second fiber to activate another sensor) in addition to the classical positive and negative electrode.

The long term goal is that the 2030+ battery will no longer be a black box. This vision needs to be addressed hierarchically at both the component level and the full system level. Injecting smart functionalities into the battery cell can be made in several different ways. It enlists possible integration and development of various sensing technologies to transmit information in and out of the cells. Sensors that can measure multiple parameters at various locations within a cell (spatially resolved monitoring) are especially important. Parameters such as temperature ($T$), pressure ($P$), strain ($\varepsilon$), electrolyte composition, electrodes breathing ($\Delta V$), and heat flow with high sensitivity are valuable options.

The introduction of fluorescence or IR probes with optical read-out for the identification of chemical species is one option. This means that in addition to the classical + and – poles, there is also an analytical output which can transmit and receive signals. To ensure the successful implementation of such embedded sensors into a practical battery cell the adaptability of any of the sensing technologies must be considered. The target 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 in order to develop intelligent responsive battery management systems. This needs to be done in collaboration with the BIG-MAP part of this roadmap.

In this chapter, we first review the current status of sensors and sensing activities within the field of batteries so as to identify the remaining scientific, technological and systemic challenges. Strategies to alleviate them within the context of BATTERY 2030+ are discussed and highlighted prior to the presentation of our ten years’ road map with specific milestones to bring these new concepts to flourish; up to the ultimate goal of creating highly reliable...
batteries with ultrahigh performance and long-life. The higher the capacity in a battery cell, the more important it will be to ensure safety and long life of the battery.

4.3.1. Current status

Over the years, a lot of fundamental studies have been done on different battery chemistry by using sophisticated diagnostic tools such as X-ray diffraction, nuclear magnetic resonance (NMR), electron paramagnetic resonance (EPR) or transmission electron microscopy (TEM), which can ideally operate in situ and even operando as the battery is cycled[71]. Although quite spectacular, these analytical techniques rely on specific equipment and cells and cannot be transferred for analyzing commercial cells. In contrast, Li-distribution density and structural effects were recently imaged in 18650 cells but these imaging techniques rely mainly on large scale facilities with limited access[72]. Notable progress has been made over the years towards instrumental miniaturization, so that bench-top X-ray diffraction units, scanning electron microscopes and portable impedance (and even NMR) spectrometers exist, but we are still far from producing the test units needed to monitor batteries in their end application. Hence, the need for a paradigm shift towards monitoring the battery functional status in real time is still open.

Determining the state of charge (SoC) of batteries is a problematic issue, nearly as old as the existence of batteries, hence the wide variety of ingenious monitoring approaches developed over the years leading to numerous patents covering various sensing technologies (Figure 10). For decades, this sensing research was mainly devoted to the Pb-acid technology in order to make it more reliable and friendlier to customers. Through this period, a great advancement was achieved with the implementation of electrochemical impedance spectroscopy (EIS) as an elegant tool to evaluate the evolution of the cell resistance upon cycling of the Pb-acid batteries, hence enabling an estimate of their state of health (SoH).[73] As such, portable EIS devices were commercialized and used in the field of transportation, and as back-up units for telecommunication, to find faulty batteries within a module. Such devices still exist but suffer from their poor reliability (< 70%). Overall, SoC monitoring still remains highly challenging. Presently, there is no accurate solution. Today estimation of SoC relies on a combination of direct measurements such as EIS, resistance, current pulses measurements, coulomb counting, and open circuit-voltage based estimations.

As batteries become more and more the heart of our daily lives, there are increasing demands for highly reliable and long-life batteries. This has revitalized battery sensing activities with the emergence of novel approaches to passively monitor the effects of temperature, pressure, strain, ΔV of the SEI dynamic via diversified and non-destructive approaches relying on the use of thermocouples, thermistors, pressure gauges, 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 and missing internal chemical/physical parameters of paramount importance for monitoring batteries lifetime. Thus, implantable sensors gain increasing interest with a predominance for optical sensing (Figure 12). Recent publications have reported the positive attributes of Fiber Bragg grating sensors (FBG’s) and others to: i) accurately monitor (T, P and ε) upon cycling, ii) achieve cell temperature imaging, and iii) estimate the battery SoC without interfering with the cell performance. Time has come to move out of this 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 packs and modules have been tried (Figure 12), and it is not the scope of this review to list all of them but rather to highlight the ones having the greatest chances to succeed at the battery cell level.

Temperature sensors
The single knowledge of surface temperature at one location of a battery cell has long been used to validate thermal battery management system models (TBMS). Temperature sensors fall into four main classes: resistance temperature detectors (RTD), thermally sensitive
resistors (thermistors), thermocouples, and fiber Bragg grating optical sensors (FBGs). These differ in their accuracy and their easiness to be positioned within the cell. Thermistors, because of their thicknesses (1 mm), are solely positioned on the top rather than at the surface of the cell as opposed to (100µm) RTD’s.[74] Interestingly, longitudinal surface variation of cell temperature during operation can be mapped with an accuracy of at ± 1°C by screen-printing of thermal sensors arrays on the surface casing of 18650 cylindrical cells. However, the scarcity of information regarding the inside of the cell hinders the integrity of today’s TBMS model, leaving their accuracy and predicting capabilities questionable. Simplified attempts to alleviate this issue have consisted in implanting thermocouples within 18650 and pouch cells, and the successfully electrocardiogram of a 25Ah battery was realized by embedding 12 thermocouples at the specific locations within the cells, and 12 additional ones located at the same position but at the surface of the cell.[75] As such, temperature contours within the cell could be plotted, providing valuable information to validate thermo-electrochemical models. A drawback pertaining to this approach resides in the positioning of the various thermocouples and their wiring without affecting the tightness of the cell and its performance. A friendlier way to assess temperature contours and identify hot spots within the cell enlists infrared thermography, but this technique suffers from poor spatial resolution together with limited accuracy in temperature besides background noise.

**Gauge sensors (ε,P)**

Besides monitoring temperature, methods to sense intercalation strain and cell pressure are equally critical techniques for controlling the SEI dynamic which affect the SoC as well as SoH of batteries. Early experiments have relied on the use of *in situ* strain-gauge measurement to probe, for instance, the total volume change during charging and discharging of Ni-Cd batteries. This work was extended to the study of commercial Li-ion LiCoO₂/C cells, and others, to measure strain associated with phase transition as well as to quantify delays in the cell volume variation as a function of the cycling rate. Recently, *via* a strain sensor placed at the surface of the cell, J. Dahn et al., simply demonstrated that the irreversible volume expansion caused by SEI growth could be detected by *operando* pressure measurement in addition to the establishment of a correlation between capacity retention and irreversible pressure increase.[76] The simplicity of such an approach which solely relies on the use of external sensors constitutes its asset. However, placing strain sensors at the cell surface fail short in providing spatial information which is critical for improving SoC and SoH batteries.

**Electrochemical sensors**

Electrochemical sensors are mainly used to sense battery chemical aspects such SEI growth, redox shuttle species, and metal dissolution. Recently, Dahn’s group has convincingly demonstrated the feasibility of using differential thermal analysis (DTA) as an elegant way to track substantial changes in the electrolyte composition as a function of the state of life of the battery [77]. DTA of the entire pouch is envisioned as a non-destructive method to correlate the melting point of the electrolyte to the cell’s state of health. Therefore, it remains an *ex situ* technique with no chances of miniaturization nor of being used to track batteries in real applications.
Typically, electrochemical (voltammetric, amperometric) cell/system used in the laboratories can be viewed as electrochemical sensors to detect various species, but an inherent drawback for battery sensing is miniaturization issues. This is changing owing to recent advances in the field of bio-physics/chemistry so that electrochemical sensors are now extremely suitable for miniaturization down to micro- or even nano- dimensions using several mechanical, chemical and electrochemical protocols to prevent environment artefacts (convection, etc.). Thus, the combination of advanced electrochemical (pulse) techniques and unique suitability for electrode/sensor miniaturization and electrode modification provides excellent podium for designing new powerful detection Microsystems which could be conveniently incorporated into batteries provided that remaining materials aspects can be solved.

A persisting challenge in electrochemical battery diagnostics is the development of effective and (electro-) chemically stable and durable (quasi-) reference electrodes that can be used in voltammetric/amperometric and/or potentiometric detection regimes. Reference electrodes (RE’s) have been of paramount importance in the understanding of various battery system chemistries at the lab scale where a few tens of cycles are usually sufficient to unravel failure mechanisms and other limitations. They enable (i) the distinct contribution of each cell component to the overall battery performance, (ii) the correct interpretation of current and voltage data with respect to the components, and (iii) the study of reaction mechanisms of individual electrodes. However, there are difficulties in i) having RE’s of well selected chemical composition for ensuring chemical inertness to the cell environment and ii) defining both the proper RE geometry and location with respect to the other cell components which depend upon the cell configuration to prevent experimental artefacts. The use of RE’s for battery sensing is therefore appealing. However, it must be realized that as of today reliable, user-friendly, chemically stable, long lasting and free of artefact cell configurations do not exist. Solutions are awaiting to be found.

Optical sensors

The Fiber Bragg Grating sensors (FBG’s) which correlates the wavelength dependence of the emitted signal with local temperature, pressure and strain are by far the most studied. Few research groups have shown how FBG’s could be used to provide a thermal mapping of battery pack.[78] Moreover, PARC (a Xerox company) has demonstrated the feasibility to obtain highly-performing lithium-ion pouch cells for EV’s applications having embedded FBG sensors attached to the electrode while not observing major adverse effects of the embedded fiber on the cell life for at least 1000 cycles.[79] Based on accuracy of the strain measured using FBG’s, the SoC was estimated with less than 2.5% error under different temperature conditions and under dynamic cycling. Equally, the authors could predict the cell capacity up to 10 cycles ahead with approximately 2% error. However, a difficulty with FBG’s is to simply decouple pressure and temperature.

A solution to this decoupling issue has been provided by the arrival of microstructured optical fibers (MOFs) - also known as photonic crystal fibers (PCFs)[80]. Unlike FBG’s whose functioning relies on a change in refractive index between core and cladding to obtain total internal reflection of light, MOFs achieve total internal reflection by a manipulation of
their waveguide structure enlisting air holes within the fiber core whose patterning determines the specific properties of MOF’s sensors. Hence, via a wise design of the air-hole pattern, MOFs offer the feasibility to measure temperature and pressure independently with a single fiber. However, MOF’s fabrication is still in its infancy.

**Nano-Plasmonic Sensing (NPS)**, introduced as late as 2017 to the field of batteries, has the advantage to focus, amplify and manipulate optical signals via electron oscillations, which are known as surface plasmons (SPs). NPS technology relies on the shift in the wavelength of the plasmon resonance peak, due to a change in the refractive index (RI) of the surrounding medium in the closest vicinity (< 100 nm) of the sensor surface. These sensors can then be used for *operando* monitoring of physico-chemical phenomena occurring on the nano-scale such as SEI growth, lithium intercalation/deintercalation or local ion concentration variations.[81] However, the making of such sensors requires the deposit of a metallic plasmonic nano-structure on top of the fiber, whose physico-chemical stability upon cycling in presence of electrolytes remains unanswered.

**Acoustic sensing.** Batteries are breathing objects that expand and contract upon cycling with volume changes that can reach up to 10%. This leads to important mechanical stress inside the battery’s materials (cracks) that can generate acoustic signals. The “listening” and analysis of 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 is used to monitor numerous types of battery chemistries (e.g. Pb-acid, Ni-MH) and more recently was implemented to the study of Li-ion batteries during the formation stage. However, AE suffers some important limitations relating to the minimum threshold stress required for generating acoustic waves as well as the lack of space recognition as a sensing technique. In contrast AE is a very effective for studying the formatting step of batteries; detect operation conditions leading to an excessive stress to the battery’s materials or the early signs of abnormal behavior that could lead to safety issues. Such limitations were partially limited by measuring the speed of ultrasonic acoustic waves generated by piezo-electric transducers propagating through the battery. Using such an advance, researchers have exploited the physical properties of the acoustic signal transmitted (amplitude, frequency distribution, etc.) to estimate the SoC of Li-ion batteries[82]. **Nevertheless, a remaining limitation of acoustic interrogation technique is the copious wiring that** is 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 monitor of smarter batteries. However, for this to happen we need to master the communication of the sensors with BMS systems. Thus, the communication interfaces of the sensor must be viewed as an integrate part and has to be taken into account at the co-design of sensor and cell. A challenge is rooted in having an autonomous reaction of the BMS to the sensor information received, which is based on proven cell and battery models and may even be AI-based. To bring this fascinating field to fruition, subsequent advances dealing with both hardware and software are needed. This is discussed next and will be a direct link to the methods developed in the BIG-MAP part of BATTERY 2030+. 
4.3.3. Advances needed to meet the challenges

Our proposed disruptive approach to meet these challenges is to inject smart embedded sensing technologies and functionalities into the battery **capable of performing spatial and time-resolved monitoring of changes that are detrimental for battery life.** This long-term vision needs to be **addressed hierarchically on the component level 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 which relies on either on optical, electric, thermal, acoustic or even electrochemical concepts. **To transmit information in/out of the cells.** Sensors that can measure multiple parameters with great accuracies such as strain, temperature, pressure, electrolyte concentration, gas composition and to the ultimate access the SEI dynamic must be designed/developed. For successful implementation of the sensing tooling into 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 battery environment, we need to develop sensors with innovative chemical coatings having extremely high chemical and thermal stability. Equally, the integration-injection of sensors in the battery will necessitate a reduction of their size to a few microns to be fitted into the thicknesses of electrodes- separators, and hence not affect the cell performance. Manufacturing-wise a pressing goal is to make sensors an integral part of the battery, and not simply as an addition. Different strategies can be applied, for instance as has been done for thermistors, printing processes for sensors fabrication opens new opportunities for integration of sensors outside but also inside batteries cells as well as on batteries components for **in situ** measurements. Such new avenues will have to be explored in conjunction with the BATTERY 2030+ activity on manufacturing and recyclability. Moreover, an ultimate challenge is to approach wireless sensing to bypass the connectivity issues associated with the implementation of today’s sensors whichever they are, provided that the noisy environment of the battery enables wireless communications. It must be realized that the addition of wires into the cell could make manufacturing so expensive that it could not be outweighed by sensor’s benefit. A first step towards less wiring could consist in the development of novel sensors capable of monitoring several parameters in one, as for instance coupling FBG’s, MOF’s and NPG’s functions on a single sensor while not upsetting the cell performance. Equally, different Bragg gratings could be inscribed into the same fiber to allow for so-called multiplexed measurements. Distributed sensing as offered by MOF’s could be a possible solution as well, if we master their design. Lastly, cells must be used to develop sensing concepts, anticipation that findings could be implemented to modules and battery packs.

To ensure societal impact, our approach must be systematic and include the tri-connection battery pack, BMS and application. Sensing will provide a colossal amount of data that is a blessing for artificial intelligence (AI). Wise injection of this data into BMS is another indispensable aspect to consider. Obviously, this part will greatly benefit from the AI pillar of BATTERY 2030+ so that transversal efforts are being planned and will be highly encouraged for developing sophisticated BMS and TBMS systems based on the synergy between AI and sensing.
4.3.4. Forward vision

Within a ten-year horizon, the development of new sensors with high sensitivity and accuracy along with 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 with a real active connection to the self-healing function, is the objective of the roadmap for the BATTERY 2030+. Needless to say, reaching this long-term vision of smart batteries includes several research facets with their own fundamental challenges and technological bottlenecks. Among the foreseen milestones are:

**In 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 the feasibility to assess in vivo different relevant phenomena (e.g., interface dynamics, electrolyte degradation, dendritic growth, metals dissolution, materials structure change). Monitoring the normal-abnormal evolution of the battery key parameters during cell operation and defining the proper transfer functions from sensing to BMS; Increase the operational temperature window by >10% through on-the-fly sensing.

**In medium term:** Miniaturisation and integration of the (electro)chemically stable identified sensing technologies with multifunction at the cell level but also in real battery modules, in a cost-effective way, compatible with industrial manufacturing processes; Establishment of new self-adapting and predictive controlled algorithms exploiting sensing data for advanced BMS; Integration of sensing and self-healing in BIG-MAP; Demonstrate reduction in electrode overvoltage for multivalent systems by >20%; Increase the accessible voltage window by >10% for Li-ion

**In long term:** Master the communication of the sensors with an advanced BMS relying on the new AI protocols by wireless means 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 so as to reach smart batteries relying on an integrated sensing-BMS- self-healing system.
4.4. Integration of smart functionalities — self-healing

The development of substantially improved rechargeable battery cells is a must in the transition towards clean energy and clean mobility [83]–[90]. Besides the absolute need of developing sustainable batteries, our increasing dependency on batteries calls for great efforts in ensuring their reliability [91], [92]. Detection of irreversible changes (sensing) is a first step towards better reliability. However, to really ensure reliability the cell should be able to automatically sense damage and also to reinstate the virgin configuration together with its entire functionality [71]. A self-healing program must thus be developed hand in hand with the sensing one. The ability to repair damage spontaneously is an important survival feature in nature as it increases the lifetime of most living organisms. So a burning question is raised: can we try to mimic natural healing mechanisms to fabricate smart and long-life batteries [93]? Biological systems offer a great diversity of self-healing processes with different kinetics, such as stopped bleeding (minutes), skin wound healing (days) and repair of broken bones (months). Nevertheless, the desire to accelerate curing time has led to the emergence of a vast and multidisciplinary field in medical science called “regenerative engineering” [94].

As in the medical field which heavily relies on the vectorization of drugs for treatment of diseases [95], [96], it will be essential to develop, within the battery, a tool for the on-demand administration of molecules that can solubilize a resistive deposit (as the solid electrolyte interphase layer) or inject self-healing functionalities, to restore a faulty electrode within the battery (Figure 11) [97]–[101]. This constitutes another transformational change within the battery community as nearly nothing has been done on this topic.

Sensing and self-healing functionalities are intimately linked. Our ultimate vision of smart batteries integrates both these two functions. Signals detected from the sensors will be sent to the battery management system and analyzed, and in case of problems, the BMS will emit a signal to the actuator for triggering the stimulus of the self-healing process. This game-changing approach will bring maximize QRL as well as user confidence and improved safety.

This far-reaching goal is not only ambitious but also motivating since there is no coherent European research effort on battery self-healing. Hence the need to create this community by bridging different disciplines, knowledge and practices. An intimate synergy between sensing/monitoring-BMS-self-healing will secure success (Figure 13), hence enabling Europe to take worldwide leadership in battery self-healing.
This chapter attempts to review the current status of self-healing activities within the field of batteries and to identify the challenges. The proposed strategies to alleviate these challenges will be presented as well as the 10-year roadmap.

4.4.1. Current status

Self-healing mechanisms can be classified either as autonomous, when there is no need for any intentional healing stimulus, or as non-autonomous, when additional external stimulus (e.g. heat, light, pH etc.) is needed [102]. In both cases the components of the healing process need to be highly reactive to achieve fast and efficient reactions with solid surfaces. Due to this fact very few self-healing approaches within the battery field have yet benefited from the general strategies and formalisms well established for human bodies. Copying nature’s strategy that rely 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, host-guest or Van der Waals interactions [103], [104]. Functionalized and flexible polymers with chemical compatibility with the battery components have been developed, with reactive species produced in the material in response to damage. Another self-healing approach, barely applied until now in the battery community, uses microcapsules hosting healing species. These need to stay active upon their release, which is triggered by a stimulus [105]. A plethora of self-assembling materials [106]–[109], and bio-inspired mechanisms pertaining to the field of supramolecular chemistry and biology, have also been tried to exploit radically new smart functionalities for either intrinsic or extrinsic self-healing processes.

In order to protect batteries from thermal management (the most common failure mode) different approaches that include thermo-switchable polymers with thermal self-protection integrated into the electrolytes and current collectors have been pursued [110]–[112]. Moreover, and specific to batteries, the identified self-repairing chemical tools must be highly resistant against the harsh oxidizing/reducing chemical environment of the cell. This has slowed down the introduction of self-healing approaches in the field of energy storage.
However, this is rapidly changing as witnessed by a few recent studies dealing with the incorporation of self-healing functionalities into batteries and super capacitors. In conclusion, the field of battery self-healing is rapidly gaining momentum as shown in Figure 14.

**FIGURE 14.** Schematic representation of self-healing mechanisms in batteries material [27].
4.4.2. Challenges
Self-healing activities within the field of batteries have mainly targeted the auto-repair of electrodes to restore conductivity, as well as functionalization of membranes to regulate ion transport or minimize parasitic reactions. Some of these aspects are addressed in more details below.

Restoration of electrodes conductivity
The restoration of electrical properties after damage is of paramount importance in energy storage devices. Great hope is placed in the development of healing systems that use a conductive material that creates physical and electrical integrity between crack/fracture facets, coating shells, electrodes-current collectors and so on. The first studies on the self-healing of conductivity used urea-formaldehyde microcapsules, filled with carbon nanotubes (CNTs) dispersed in chlorobenzene or ethyl phenylacetate, to provide both mechanical (solvent) and conductivity (CNT) healing. These microcapsules were tested by embedding them in layers of epoxy above and below a glass slide patterned with gold lines. Sample fracture resulted in the conductivity being lost as a crack formed in the gold line. The microcapsule bursts when physically damaged, leading to the release of carbon nanotube suspensions which restore the conductivity after a few minutes (Figure 15) [105], [113].

Figure 15. Testing self-healing of the gold line after a damage [29].

Other conductive chemical systems were similarly encapsulated and tested, including among others carbon-black (CB) dispersions [114], [115]. These are very attractive since CB is already used as a conductive additive in graphite anodes. Such dispersions in combination with co-encapsulated poly- (3-hexylthiophene) (P3HT), were successfully used to restore conductivity in cracked silicon anodes. This increases the chances of developing practical silicon anode for a lithium-ion battery which are prone to lose integrity because of their nearly 400% volume change during lithiation. Inherent drawbacks to this elegant approach are its irreversibility and the amount of required electrochemically dead microcapsules which penalize the cell energy density.

Further dealing with Si anodes it is also worth mentioning. Wang’s early work reported a polymer coating consisting of a randomly branched hydrogen-bonding polymer (Figure 16), which exhibited high stretch ability and sustained the mechanical self-healing repeatability that helped the Si anode to withstand large volume expansion after many cycles [104], [116], [117]. An extension of this concept by the same group has led to the design of electrodes with
a 3D spatial distribution of the same self-healing polymer into Si anodes for ensuring a better adhesion, giving high cycling stability [118]. Besides hydrogen bonded polymers, self-healing binders based on several other supramolecular interactions have been employed as well for Si anodes [119]–[123] and S cathodes [124]. Therefore, long testing is sorely needed to fully evaluate the practicality of these approaches.

Another concept of auto-repair that was developed by Deshpande et al. [125] relies on the use of liquid metal (LM) anodes; that is metallic alloy (Li$_2$Ga) having a low temperature melting point so that 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. This approach was subsequently implemented to other Li-alloying negative electrodes, as well as to other chemistries. For instance, self-healing Ga-Sn electrodes [126] were shown to have excellent cycling performance (> 4000 cycles) and a sustained capacity 775 mAh/g at rate 200mA/g. Self-healing alloys (Na-Sn) were also implemented by Mao et al. [127] for improving Na-ion batteries.

Deviating from batteries, an electrically and mechanically self-healing supercapacitor was demonstrated. Its conductive electrode was fabricated by spreading a TiO$_2$ functionalized single-walled carbon nanotube (SWCNT) film onto a self-healing polymer substrate, consisting of a supramolecular network of H-bonds donors and acceptors. The broken CNT contacts after damage was repaired by the lateral movement of the underlaying self-healing polymer, thereby restoring the electrode configuration and electrical conductivity [128]. Specific capacitances 140 Fg$^{-1}$ could be achieved with the feasibility of recovering 92% after several breaking/self-healing cycles. Interestingly, the self-healing insulator polymer widely used in these studies is based on the one reported by Leibler in 2008, prepared by the supramolecular cross-linking of fatty dimer acids with urea. This polymer has often been the material of choice as it functions without the need of any external stimulus while recovering repeatedly several hundred percent of extensibility.
Supramolecular interactions frequently involve H bonding. This is not ideal to design self-healing binders for non-aqueous battery systems due to the parasitic reactions involving hydroxyl groups. This constraint is no longer present for Li-based aqueous batteries. This was exploited by Zhao and co-workers, who demonstrated a new family of all-solid-state, flexible and self-healing aqueous LIBs using aligned CNT sheets loaded with LiMn$_2$O$_4$ and LiTi$_2$(PO$_4$)$_3$ nanoparticles on a self-healing polymer substrate [129]. The assembled aqueous LIB, once cut, could be healed in a few seconds by simply bringing back into contact the two parts. Similarly, a new-generation self-healing zinc-iodine flow battery (ZIFB), which consists of a porous membrane that can absorb I$_3^-$ was reported by Li et al. [130] Basically, by overcharging the cell the I$_3^-$ contained in the membrane oxidize the zinc dendrite so that the battery self-recovers.

**Designing self-healing electrolytes**

The use of self-healing electrolytes is yet another impressive strategy applied to improve the electrochemical performance and durability of both non-aqueous and aqueous batteries. First proof of concept was demonstrated 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 with a sustained capacity of 1450 mAh g$^{-1}$ and a high coulombic efficiency [131]. In order to further improve the efficiency of Li-S batteries, Zhang et al. [132] designed self-healing electrolytes (SHEs) preloaded with polysulfides and containing auto-repairing agents so as to mimic fibrinolysis, a biological process occurring within blood vessels. Through this process, the additive agent solubilizes solid Li$_2$S, hence enabling its subsequent participation in electrochemical cycles. Li-S batteries with an optimized capacity could thereby be cycled for more than 2000 times. Lastly, dealing with aqueous zinc-ion battery (ZIBs), Huang et al. designed, via a facile freeze/thaw fabrication of poly(vinyl alcohol/zinc trifluoromethane sulfonate ((PVA/Zn(CF$_3$SO$_3$)$_2$)), an hydrogel electrolyte that can autonomously self-heal by hydrogen bonding without any external stimulus [133]. By incorporating the cathode, separator and anode into a hydrogel electrolyte matrix during the freezing/thawing process of converting the liquid to hydrogel, they could demonstrate the assembly of Zinc-Ion Batteries (ZIBs) that display full electrochemical performance recovery even after several cutting/healing cycles. This approach offers broad prospects to fabricate various self-healing batteries for use as sustainable energy storage devices in wearable electronics.

**Other self-healing strategies**

Self-healing tools, consisting thin TiO$_2$@Si yolk-shell structure with self-healing artificial SEI + natural SEI, were also designed by Jin et al. [134]. As the TiO$_2$@Si yolk-shell gets cracked, internal electrolyte was expelled due to the volume expansion of silicon during lithiation. This ensured the contacts between silicon core and TiO$_2$ shell covered with the artificial SEI. As a result, fresh natural SEI formed on both the surface of silicon and TiO$_2$ shell to connect and repair the cracks. With such a trick, coulombic efficiency exceeding 99.9% and excellent cycling stability was demonstrated.

Dendrite growth has been a long-lasting problem which has prevented the development of non-aqueous Li metal batteries, and stands out as as a technology block for development of today’s solid state Li batteries. Interestingly, Koratkar et al. succeeded in achieving a substantial self-heating of the dendrites by using a high plating and stripping current
(~9 mAh/cm\(^2\)) [135]. With a high current, they could trigger an extensive surface migration of Li that smooths the lithium metal surface, hence ensuring the homogeneous current distribution that is needed to prevent dendrites growth. So, using repeated doses of high current density healing led to lithium-sulfur batteries containing 0.1M LiNO\(_3\) which cycled with high coulombic efficiency.

Altogether, 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 performances and reliability. Although this field is still in its infancy, these studies have set the playground for new research trends while stimulating novel and exciting research activities towards Battery Self-Healing (BSH). Most of the reported auto-repair demonstrations are fundamentally elegant and appealing but far from practical use. Such a fundamental-applied gap must be closed, and this poses numerous challenges calling for innovative research and technological developments.

4.4.3. Advances needed to meet the challenges
Redox reactions occurring through the battery operation are frequently accompanied with additional reactions at the thermodynamically unfavorable interface which releases 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 at the anode surface or trigger shuttling self-discharge mechanism. Therefore, the proposition of functionalizing the separator by anchoring chelating agents to its surface which could capture dissolved transition metal ions, before they are reduced at the anode surface. Another option could consist in grafting proteins on the membrane to regulate the migration of parasitic organic species.

*Functionalized membrane*

The use of separators for grafting-anchoring trapping molecules inside their porous channels is attractive for several reasons. 1) The dissolved TM ions are transported due to diffusion and migration through the separator, what renders them available for capture by the anchored trapping molecules. 2) The porosity of the separator facilitates high specific surface area for deposition of optimized amount of traps per volume. The high amount of ion cavity sites will increase the probability for ion capture, and the amount of ions that can be captured per unit of volume. 3) The trapped molecules that are anchored inside the porous separators are far enough from the sites of electrochemical reactions, so that they are protected from negative/positive potentials that might affect their stability. 4) The separator provides an ideal host to graft molecules, that can uptake ions at room temperature, and last but not least the separator can be specifically designed with self-healing properties alike the electrodes.

Among candidates to synthetize the membrane, cyclodextrins turn out to be very promising due to their high solubility, their lipophilic inner cavities and hydrophilic outer surfaces, their bioavailability and their specific recognition ability toward small guest molecules/cations enabling them to form inclusion complexes. Moreover, specific to such cyclodextrin trapping is its temperature dependence; hence the feasibility to use temperature as a stimulus for the uptake or release of trapped species on demands. Another option, although less environmentally sustainable, lies in the use of crown-ethers or calixarenes whose highly open structure is a gift to anchor a variety of chelating ligands capable of regulating ion transports.
without risks of blockades. Moreover, their grafting procedure is not too complex. Implementing such new concept towards the design of smart separators is new and exciting.

*Polymer membranes*

Polymer membranes as solid polymer electrolytes and also under study as electrode redox active materials or components of hybrid solid-state electrolytes. Even metal coated polymeric current collectors are offered commercially. Since polymers can be formed or cross-linked in-situ they can be used themselves as mechanical healing agents within the battery cell, similarly to epoxy or cyanoacylate (i.e. super glue) resins. Moreover, they can act as template for inorganic capsules formation on a medium time scale. Since the use of polymers in batteries is virtually unlimited by use of composite components, this allows for developing self-healing strategies for most components and interfaces based on self-healing polymers. Thus, they constitute the cornerstone of BATTERY 2030+ self-healing strategies.

Supramolecular assembly may offer a unique playground at a short term scale to address 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, and could be used for battery components that can accommodate protic organic compounds. Equally, 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 pace of non-covalent interactions, but this requires further work. Lastly, the exploration of multiphasic solid polymer electrolyte systems could also allow application of different self-healing strategies whenever a stimulus can induce a mixing of domains.

*Bio-sourced membrane*

Another challenge consists in mimicking biological membranes in term of barrier selectivity, in order to control the decomposition of electrolytes so as to improve battery aging. A key milestone will be to follow, inside the battery, the electrolytes stability, with a sensitive and selective sensor at single molecular scale using the nanopore technology with an electrical detection. For this to happen, one needs to design thin and porous controlled membranes using chemistry of non-toxic and bio-sourced molecules/proteins (e.g. cyclodextrins), whose selectivity can be achieved by optimization and use of protein engineering.

*Self-healing electrodes*

The restoration of electrical properties after electrodes damage is crucial in energy storage devices. As for membranes, sliding gels made of reversible bounds could be used to control the organization of the surface and to optimize the efficiency of the battery device. The main advantage of the sliding gels in addition to the supramolecular interactions is the pulley effect along the polymer chain to adsorb the stress, permitting the reorganization of the architecture in order to come back to the initial properties. We can also use this gel as a reinforcement mechanical bandage, hence our eagerness to explore this road. Another option to explore is based on in the building of composite electrodes containing microcapsules capable of releasing healing agents by applying 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 others which are released upon shell breaking via a stimulus, is worth exploration.

4.4.4. Forward vision

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

There is no coherent European research effort today on battery self-healing in spite of the foreseen emerging opportunities that could ensure Europe worldwide leadership. This is what our BATTERY 2030+ is aiming to, by putting together an ambitious BSH roadmap that will lead to a game-changing approach enabling to bring batteries QRL to its maximum and serve as a driver to reunite a multidisciplinary community which commonly shares the same dream of developing long lasting batteries with self-healing functionalities. A few milestones towards such ambitious vision are listed below. This will be made sequentially:

| In short term: | Reunite excellent European research teams at the cross-over of various disciplines to launch the foundation of a new research community for developing self-healing functions for batteries. Engineer functionalized separators and develop supramolecular assemblies relying on H-H bonding for reversible crosslinking to repair electrode-membrane fracturing while being compatible with the targeted battery chemistry. |
| In medium term: | Wisely engineer separators with capsules holding organic-inorganic healing agents with various functionalities that can be triggered via a magnetic, thermal or electric modulus for auto-repairing while being electrochemically transparent. Determine response-time associated to stimulus actuated self-healing actions for repairing failures pertaining to electrode fracturing or SEI coarsening. |
| In long term: | Design and manufacture low cost bio sourced membranes with controlled functionalities and porosity for ion detection and regulation mimicking channels made by proteins from life science. Establish efficient feedback loops between cell sensing and BMS to appropriately trigger by external stimulus the self-healing functions already implanted in the cell. |

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5. Cross-cutting activities

The new materials and interfaces/interphases designed using the BIG-MAP approach, as well as the novel sensing and self-healing functionalities integrated within battery cells, must be able to be scalable, manufactured and recycled simply and affordably. Chapter 5.1 describes the steps to ensure manufacturability and likewise Chapter 5.2 describes the steps to ensure recyclability.

5.1. Manufacturability of future battery technologies

Battery manufacturing is a concept covering a large area. Generally speaking, and depending on the actual context, it may refer to individual cells, cell modules or battery pack. Therefore, this chapter is of particular interest to properly set the reference scenario. From a pragmatic point of view, the cell is the simplest element in the battery value chain that gathers the essential characteristics and features of a given “battery technology”. Any super structure made thereof basically comprises the engineering solutions to make such cells work in a practical environment. Accordingly, the present chapter will be focused at the cell level.

In this chapter we will apply the criteria that any material or component that inherently takes its final form and function during or after its integration in the cell will be considered as a part of the battery manufacturing process. Examples of this might be polymer electrolytes for solid state batteries that are cast from melt during the battery manufacturing process. From this perspective, this chapter relates to synthesis of innovative/breakthrough materials (see Chapter 4.1) and to the interfaces created inside the battery in the manufacturing process (see Chapter 4.2). Furthermore, we want to introduce the concept of remanufacturing, as an industrial process to transfer a used battery component in a quasi-new condition or to improve the functional conditions. This will have a future impact on the design of new cell concepts and battery modules.

The development of new materials with different properties and processing needs and requirements, along with the integration of new features, as sensors and mechanisms for self-healing will require a significant rethink of cell design, including remanufacturing issues as previously stated. The redesign of cell architecture is essential to drive both competitiveness and sustainability, while maintaining even increasing the energy density, and will play a central part in this work.

The availability of new generation of breakthrough battery materials will open a new world of opportunities for innovative battery technologies. However, broadly speaking, these new battery technologies will need to face at least two main validation phases. Firstly, they will need to prove their potential at the prototype level, secondly, the feasibility of their upscaling into industrial process level will need to be assessed. The approach will be useful at both levels: prototype as well as industrial manufacturing, and also covers cell design, understood as a necessary step between innovative materials and the actual battery technology.
Manufacturing of future battery technologies is addressed in this roadmap from the perspective of the Industry 4.0 and digitalization. The power of modelling and of artificial intelligence (AI) will be exploited to deliver digital twins both for innovative, breakthrough cell geometries, avoiding or substantially minimizing classical trial and error approaches, and manufacturing methodologies. Through fully digital manufacturing analogues will allow understanding and optimization of parameters and their impact on the final product.

Eco-design criteria, including design to allow easy disassembly for recycling of parts or materials, facilitating both at cell design and at the manufacturing level.

5.1.1. Current status
Lithium Ion Batteries (LIBs) are today’s battery technology of reference for various application purposes [136]. Other commercial battery technologies exist as well (lead acid, etc.), but, for the sake of clarity and conciseness, we will generally refer to LIBs as a reference. Keeping in mind that these differences exist and that current LIB design and manufacturing concepts do not necessarily represent the whole picture for other present or future battery technologies. They may though share some general principles regarding manufacturing issues.

Cell design
Presently cell design follows a trial and error approach, and it is limited to some standard formats (cylindrical, pouch and prismatic hard-case). Though there are some incipient activities where modelling is applied to the cell design [137], [138], which will open up new possibilities to explore new cell formats.

Battery manufacturing
Battery manufacturing is a quite well established art today. This is particularly true for LIBs, seen as the reference technology at present and in the near future. The three main phases are included: electrode production, cell assembly, and cell finishing. They all include several steps, like mixing, coating and drying, slitting, calendaring, vacuum drying and electrolyte filling [139].

In spite of this well-organized sequence of steps, current trial and error approaches at design and manufacturing should be overcome. This will include radically new eco-design criteria minimizing scrap, use of primary energy and producing zero or near to zero emissions. In this line, the current multiphysics modelling[140] can be of a great importance in battery design and manufacturing:

- Accelerate new cell designs in terms of performance, efficiency and sustainability, coupling multiphysics models to advanced optimisation algorithms in the artificial intelligence (AI) framework, as well, as inverse cell design, which represents a crucial step for autonomous battery design optimization, as it connects the desired properties to specific cell configuration, electrode compositions and material structures as targets to synthesize, characterize, and test (see Figure 17).
- Accelerate the optimization of existing and future manufacturing processes in terms of cell chemistry, manufacturing costs and sustainability/environmental impact.
More effort is although needed to develop multiscale physicochemical computational platform of the full manufacturing process chain of LIBs.

All these impressive efforts together with the rapidly growing computational and algorithmic capabilities, in particular in the field of AI, call us to go even further. The computational simulation of cell design and manufacturing process of new generation of batteries, for example, integrating interfaces discovered through the BIG-MAP concept and/or cells including sensing and self-healing functionalities, will certainly pose new exciting challenges for multiscale computational science.

5.1.2. Challenges

Current LIB manufacturing processes face numerous challenges in order to achieve efficient, reproducible and consistent production of batteries, according to high quality standards, environmental impact and economic competitiveness.

On the other hand, there is a continuous evolution within the state-of-the-art towards new technologies aiming to higher energy density, long lasting and safer batteries. In some cases the evolution may lead to a different paradigm in how batteries are designed and manufactured. To mention some examples, today’s trends in lithium-based batteries involve the use of metallic lithium anodes, intercalation thin layer electrodes, solid electrolytes, polymeric, inorganic or hybrids combining both. These and other approaches call for a substantial redesign of current manufacturing processes.

Given the disruptive nature of the concepts to be developed within the BATTERY 2030+ initiative, there is also the need to think out of the box at the cell design and manufacturing
fields. It is not easy to anticipate how future battery technologies will look like, and in consequence no one can foresee exactly what manufacturing concepts will need to be put in place. Nevertheless, there are advanced tools at the technological forefront that will certainly play a central role in the future that may well be anticipated from today’s perspective.

In this sense, the challenges faced by the battery manufacturing industries can be divided in two levels. The **first level** of challenges is related to current battery production general methodologies, with strong impact in the short-term, but that will continue challenging the implementation of manufacturing for forthcoming battery technologies. These challenges are being already tackled today, but they will probably remain an open issue for some time, needing optimization and adapting to new materials and concepts. The **second level** involves advanced manufacturing concepts and approaches for battery technologies of the future that we today only can hardly envision. This part is at the core of the scope of BATTERY 2030+, and hence central to this roadmap.

According to these two levels, the following challenges may be outlined:

**Manufacturing challenges bound to current (mostly Li ion) battery manufacturing methodologies:**

- **Overcome today’s trial and error as a general tool to fine tune current battery manufacturing processes and shorten development time.** The current process chain is highly complex and associated with very high investments. Competitive production currently requires the exploitation of economies of scale, which leads to so-called *Gigafactories* with tens of GWh manufacturing capacity. These factories are usually very specialized to chemistry and limited to a few cell formats. Despite the strong optimisation of current production lines with trial and error approach, there is still a very high quantity of material and cells, which do not comply with specifications. This makes the change to new cell chemistry and materials, but also the manufacturing of novel cell formats very difficult 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 cells is very difficult and expensive, and also limits the market launch of novel material and chemistries.

- **Difficulties to adapt/modify current manufacturing processes to accommodate next generation Innovations such as using metal foil anodes –e.g., metallic lithium–, solid electrolytes –e.g., polymer, hybrid or inorganic–.**

- **Overcome the paradigm of individual cells** Involving excess of packaging material, connections and cabling towards bipolar and other structures (design issue with significant impact in manufacturing).

- **Establish a cell design and processes to allow for component level recycling /reuse** (i.e. electrode recovery and reuse from end-of-life well performing cells).

- **Develop tools to predict the impact of processing parameters in 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.

- **Lower the general process cost** - with less solvent and energy use, reduce scraps, along with faster manufacturing especially during the formation step.
Challenges related to future battery materials and technologies arising as a result of the foreseen highly innovative batteries R+D scenario:

- **BIG-MAP to produce innovative materials/interfaces** with specific manufacturing issues: creates a need for flexible manufacturing process design strategy
- **Rapid prototyping methods** to implement design rules from BIG-MAP.
- **Introduction of self-healing materials/sensors plus** their potential need of external physical connection at cell level for activation/bidirectional communication.
- **Introduction and viable upscaling of 3D or other mesoscale composite materials in electrode and cell processing,** without affecting microstructure/functionality – will generate a need to preserve textural /functional properties.
- **Need of tools to predict the impact** of manufacturing parameters on the battery component functional properties, somewhat in parallel with the introduction of new materials and concepts at cell level.
- **Manufacturing routes** facilitating direct recycling methods preserving the structural elements of the cell (electrodes, sensors, etc.)

### 5.1.3. Advances needed to meet the challenges

In a future scenario, current trial and error approaches should be avoided and cells and manufacturing processes need to be ”smart”, giving them a digital identity creating a digital twin, which is a virtual counterpart to a physical object.

The advances needed for future cell design and manufacturing processes can be summarised as follows:

- Introduction of new functionalities, like self-healing materials/interfaces, sensors or other actuators, cell eco-design and alternative cell designs.
- Flexible manufacturing processes and flexible, high precision modelling tools for the optimization of processing and conditions and machine parameters. In this way, human labour, trial and error, and waste products will be minimized; development of real-time models for the processing of electrode pastes and the performance in the cell (digital twin for cell manufacturing).
- Development and validation of multiphysics and multiscale models on cell manufacturing processes capable to provide accurate understanding on each steps of the process.

### 5.1.4. Forward vision

The main goal of the digital twin models designed for cell manufacturing processes is to solve physical issues faster by detecting them earlier in the process, and to predict outcomes to a much higher degree of accuracy (see Figure 18). Additionally, their ability to evaluate performance of the equipment in real-time may help companies having value and benefits iteratively and faster than ever before.
The main benefits of this approach are as follows:

- Gives new optimum cell design for specific applications / cell chemistry.
- Develops new manufacturing methodologies.
- Development of models which calculate ultimate manufacturing parameters.
- Improvement of battery performance (power and energy density, etc.), through advanced design.
- Faster processing – fast manufacturing & prototyping.
- Improved quality control
- Provides an appropriate link to cell design, materials and BIG-MAP.

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

In the long-term, 10 years and beyond, full maturity of the methodology is expected, closing the loop by means of integration of the cell design and manufacturing design sub-loops with interface, with BIG-MAP as a fully autonomous system (using AI) (see Figure 19). Based on the BIG-MAP output, an automated cell prototype will be generated. In addition, some parts of this methodology can be progressively made available to the industry, before the full package will be available as a commodity to a new state-of-the-art.
Potential impacts on this approach:

- Accelerate the discovery of new cell designs and manufacturing processes.
- Reduction of the development time and cost for new battery cells.
- Reduce battery research and innovation (R&I) cost.

Potential risks on this approach:

- Data management (usable; accessible; integrated; curated).
- Data harmonisation (standards)
- IPR management (data ownership).

In short term: This would be done starting from state-of-the art information, and focus will be the battery cell design methodology. This would include the improvement of simulation tools such as – multiphysics models- with the goals of reducing the computational burden and implementation of current AI techniques through deep learning and machine learning methods for cell design..

In medium term: Input is expected to come from BIG, MAP, sensing, self-healing, recycling and other innovation areas that would be integrated into the process; The methodology will be
adapted to manufacturability of new battery technologies, with the launch and implementation of the AI driven methodology to manufacturing after the developments made at cell level design: Modelling -> AI -> Manufacturing including new techniques, as well as the creation of digital twin of a cell manufacturing process; Scalable battery chemistries, e.g. multi-valent and organic; Demonstrate transferability of established BIG-MAP concept to alternative battery concept, e.g. flow batteries.

In long term: Full maturity and implementation of the overall AI-driven methodology, by integrating cell design sub loops that converge in holistic prototype development, as a fully autonomous system nourishing from BIG-MAP. This methodology that will contribute to the foundation of a new state-of-the-art, developed as a commodity, will be progressively deployed to the industry and academia.

5.2. Recyclability

The development of battery dismantling and recycling technologies with high efficiencies well beyond the EU Battery Directives targets of 50 % for most battery technologies is essential to ensure the long-term sustainability of the battery economy by year 2030. This calls for new, innovative, simple and low-cost processes targeting a very high回收率 rate, low carbon footprint and economic viability. This will ensure a rather direct recovery of the active materials and single, instead of multistep, approaches. Furthermore, the new materials, interfaces/interphases and cell architectures envisioned in BATTERY 2030+, call for new recycling concepts, such as reconditioning or reusing electrodes and vice versa. Industrial participation will be brought early on board. To pave the way for such a shift, there will be a direct coupling to material suppliers, cell and battery manufacturers, main applications actors and recyclers to integrate the constraints of recycling in the 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, the BATTERY 2030+ roadmap will promote a circular economy with reduced waste, low CO\textsubscript{2} footprint and more intelligent use of strategic resources.

Implementation of designs for sustainability and more specifically designs for recycling is to be integrated in the algorithms for automated materials discovery (the input parameter can be the criticality of the raw materials, their toxicity, reduction of the number of different elements and other socio-economic aspects).

5.2.1. Current status

The battery recycling industry has known a significant development in EU following the implementation of the Batteries Directive (Directive 2006/66/EC) that introduces the Extended Producer Responsibility (EPR) for battery waste. The directive enforces 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 environmental costs associated with goods throughout their life cycles into the market price of the products. In addition, the EU has issued a number supporting and guidance documents and
the Recycling Efficiency regulation, specifying minimum requirements for the batteries recycling processes, according to the battery chemistries. According this regulation, the recycled content shall achieve: **65% in weight for the lead-acid batteries, 75% in weight for the nickel cadmium batteries and 50% in weight for all other batteries.**

Currently, pyrometallurgy is the most applied method. After potential dismantling and sorting in "categories" according to the 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 a variation or combination of different individual steps, recycling processes (or schemes) is currently classified into the processes and schemes in Figure 20.

![Figure 20. Recycling processes and schemes.](image)

### 5.2.2. Challenges

The development of closed material loops in respect 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 for all cell components to increase sustainability.

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. The latter decreases in addition the dependency of the EU on critical metal imports.

The consideration of life cycle thinking including resource extraction, manufacturability, use phase and reuse/recycling needs to be integrated within the design phase of new battery
systems to increase the overall sustainability. In the following, present challenges and the challenges foreseen for the mid- and longterm are listed.

**Present challenges**

- Battery collection targets need to be reached at end of life (Battery Directive) which seems to be less of a problem with automotive than with portable batteries. Many issues are related to collection and transportation of spent batteries.

- Batteries are complex products: micro-components, embedded electronics, etc…: no available processes for efficient components separation exist today which cause high recycling costs. Quality of the recycled products could be a hurdle for a closed loop recycling.

- Labeling of cells and batteries are necessary to sort mixed battery types and enable in this way a highly efficient recycling process.

- Especially EV automotive battery systems are designed for high safety and their dismantling poses a huge challenge to efficient recycling processes.

- The limited and decreasing value of the active materials of lithium batteries when compared to the cost of recycling pushes towards “direct” recycling processes: the demonstration of the economic benefit of these processes will be a challenge. “Direct recycling” refers to a novel recycling approach for batteries, in which the high value anode and cathode active powders and other components are recovered as such from spent cells, separated from each other and from the other recoverable materials and reconditioned to battery grade materials.

- Batteries active materials are degrading over life: i.e. structural changes in the crystalline structure of cathode materials of Li batteries may be irreversible, limiting the possibility to recover without “reconditioning” process restoring the expected level of quality and functionality. These “reconditioning processes” are not available now.

- Methodological Challenge: economic, ecological and social impacts of emerging batteries must be analysed and estimated in a prospective manner. All material, component, cell developers, recyclers and other stakeholders need to work interdisciplinary together, to reach the shared visions of new battery systems.

**Specific short/midterm challenges:**

- The number of battery chemistries placed on the market is increasing: multiple Li-ion chemistries will make specific recycling processes more difficult: the sorting quality will become a major challenge to overcome and to get specific processes applicable for components recovery. Standards for identification are important on battery and cell level to overcome these challenges.
• New battery technologies seem likely to enter the future markets e.g. solid state batteries, lithium-sulphur batteries, redox flow batteries and metal-air in mobility and stationary applications. Proposed new recycling processes need to cope with all these chemistries (and related BMS) and new process challenges will be created e.g. the presence of Li metal will affect safety aspects in the recycling processes. Processes may have to be redesigned, e.g. towards inert gas atmosphere, depending on the battery type.

• Following the large quantities of EV batteries available on the market, new business cases are appearing: re-use of battery modules or battery 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 state, and in a more mixed state. In addition, although pursued the global battery standardisation cannot be expected, due to the multiple applications placed on the market: chemistry identification and quality sorting will become even more challenging. The required level of expertise can only be expected from advanced artificial intelligence development complementing more traditional recognition means like labelling and visual observation.

• The level of attached information to the batteries will increase (first through more and more sophisticated BMS, then possibly at local level with information from sensors): processes to handle these innovations during the recycling phases will have to be developed. On the other hand, such advanced data will provide valuable input for second life applications and options to exchange single (aged) battery cells in a battery pack.

• The huge amounts of to be recycled battery systems/ modules will require enormous logistical efforts and their transportation will significantly increase costs, safety issues and CO2 footprint. Novel decentralized collection and recycling processes/ units need to be established. Societal Acceptance issues need to be considered.

• Legislative framework must be established to foster/ safeguard a sustainable design, including design for recycling.

Tentative longer-term challenges

• Big volumes of spent batteries will require a transformation of the recycling plants and a move to highly automated processes from sorting and dismantling down to the recycling itself: plant generation 4.0 for recycling will need important investments. Innovation will be needed to demonstrate highly flexible but economically feasible processes for all the steps of the recycling enabling the treatment of multiple sources of batteries in potentially different chemistries.

• The recycling technologies will need to recover future intelligent battery components such as sensors, “self-healing” components or any kind of “information” linked components.
• Additional circular economy business ecosystems for reconditioning and/or reusing of recycling products/materials will have to be developed and placed adjacent to the battery recycling units (decentralized if possible).

5.2.3. Advances needed to meet the challenges

It is the ambition of BATTERY 2030+ to trend to a new recycling model based on: data collection and analysis, automated pack disassembly to cell level, wherever possible investigating re-use and re-purposing, automated cell disassembly to maximally individualized components, and development of selective powder recovery technologies and reconditioning them to battery grade active materials that as such are re-useable in batteries for automotive/stationary applications, with significantly reduced logistical efforts.

The present “Eco-design preparatory study for Batteries” has the goal to provide the European Commission with a technical, environmental and economic analysis of batteries in accordance with relevant European Directives, especially the Eco-design Directive 2009/125/EC. Sustainability is addressed within this description, but social aspects are not considered. Moreover, the outcome of the study did only consider 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 will be considered in BATTERY 2030+ but also social aspects to ensure sustainability. Furthermore, the proposed approach will be technology open to address any innovative developments.

BATTERY 2030+ aims to provide the base of a holistic sustainable battery design starting from the raw and advanced materials, design for manufacturing and the recycling thereof (provide criteria and requirements to BIG MAP and sensing functionalities and vice versa for enabling high efficiency recycling, recovering Critical Raw Materials and minimising carbon footprint). Focus is not only on the use phase, but on the whole life cycle (life cycle sustainability) by a prospective Life Cycle Assessment (LCA), contributing by defining rules and standards for the recycling part of the loop.

BATTERY 2030+ ambition is to develop a ground-breaking new recycling process compared with the state-of-the-art. Current recycling flow in pyro- and hydro processes is summarized as shown in encompassing multi-processing steps (Figure 21):
Based on a novel integrated approach for recycling designed materials (as developed in the BIG MAP pillar) and sensoring technologies (as developed in the Sensor chapter), BATTERY 2030+ will come up with a new model based on: (Figure 22)

- data collection and analysis (from labels, BMS, sensors…)
- modern low carbon footprint logistics concepts including decentralized processing
- automated pack disassembly to cell level
- wherever possible investigating re-use and re-purposing
- automated cell disassembly to maximally individual components
- development of selective powder recovery technologies and reconditioning them to battery grade active materials that as such are useable again in batteries for automotive/stationary application. Where not possible, precursor synthesis is envisaged eventually with composition adjustments.
- international collaboration to be stimulated and developed.
Concluding over a time frame of ten years, a circular model will be developed, incorporating specific R&I actions, such as preparing a battery design for maximum longevity, considering re-calibration, refurbishing and the suitability for second life applications and multiple usages. Integrated sensing and possibly self-healing concepts can be used to identify damaged/aged components and prepare for their reuse. It will also include the development of concepts for the traceability especially of critical raw material (CRM) throughout the entire cell life, as well as automated cell sorting and evaluation and development of efficient, single step, cheap and sustainable processes to recover valuable and critical materials. Artificial intelligence and sorting equipment will be required to be applied in selective recycling processes, but also versatile processes applicable to any battery technology will be looked for: the same approach to maximally recover battery components will be targeted even in case of chemistries such as metal-air and others.

5.2.4. Forward vision

The new process for recyclability will be the basis of a series of R&I actions with the main purpose to have Direct Recycling implemented in the long term (see Figure 23).
FIGURE 23. The 10 year roadmap for recyclability within BATTERY 2030+.

Would the material/components not be suitable to be reconditioned to battery grade because of e.g. structural or purity constraints, a fall-back alternative in the last stage of the new process could be to convert them to precursors with an eventual change of composition ratio’s anticipating future chemistry changes and new generation materials

**In short term:** Start building the integration of design for sustainability and dismantling, develop a system for data collection and analysis, develop technologies for battery packs/modules sorting and re-use/re-purposing and start the development of automated disassembly to battery cells. New tests to be developed for rapid cell characterisation.

**In medium term:** Automated cell disassembly into individual components will be developed as well as sorting and recovery technologies for powders and components and their reconditioning to new active battery grade materials advanced. Recovered materials will be tested in battery application. Predicting and modelling tools for re-use of the materials in a secondary application are to be developed. Relative to current process, recovery rate of
Critical Raw Materials will be significantly improved (e.g. with recovery of graphite) and energy and resource consumption distinctly better.

**In long term:** A full system for Direct Recycling will be developed and qualified; the system will be economical viable, safe and environmentally friendly and witness a lower carbon footprint than the current processes.

**Impact**

Recycling of lithium-ion batteries from vehicles is still a developing business with large volumes expected to be recycled already onwards 2030. Since recycling is a cost-intensive industry, due to the current low volumes, recyclers struggle to find the best balance between economics and meeting the recovery targets, resulting in the industry not yet focussing enough on high efficiency and low emissions. BATTERY 2030+ Recycling Program will prepare the future to be ready to treat the expected large volumes in a responsible, sustainable and economic viable way.

6. **Other research areas to address in a large-scale research program**

This chapter is work in progress and will be completed in the final version of the roadmap. The BATTERY 2030+ community welcomes new ideas and comments.
Appendix 1 - The position of BATTERY 2030+ in an international context

Many of the existing international roadmaps target specifically the automotive sector. In these roadmaps, the focus is strongly on lithium-ion and lithium based batteries (solid-state, lithium-sulfur, lithium-oxygen, etc.). The roadmaps for energy storage in general, show a broader approach where also other chemistries such as sodium-ion batteries and redox-flow batteries play a role. Very few of the roadmaps if none contain the multivalent batteries (magnesium, calcium, aluminium, etc.) that are more and more studied in long-term basic research programs due to their promising high volumetric capacities.

Energy density and cycle life are important parameters for both transport sector and for large-scale storage. In addition, batteries for electric mobility have stringent requirements when it comes to power density and total cost, whereas batteries for stationary energy storage need to minimize the cost per unit of stored energy per cycle. The need for batteries with long durability that are safe are also important aspects. These parameters are present in many roadmaps. Another distinction is the one between energy-optimized batteries with the primary aim of storing energy (E) and power-optimized batteries that should provide short-term power (P).

The countries, beside the European SET-PLAN, that have clear roadmaps formulating long-term concentrated efforts are yet just a few of the larger nations. Here we will give a short presentation of the ones from China, India, Japan, and US to give a broader perspective to the ambitions of BATTERY 2030+.

China is now the country publishing most scientific papers in the world on batteries. Of the top ten institutions in the world in publication numbers (not quality) nine are from China and then Argonne National Laboratory in US is number five of the ten.

China defines two parallel research and innovation strategies: an evolutionary strategy and one revolutionary strategy. The evolutionary line is focusing on optimizing existing vehicle energy powertrain systems with battery studies including improved battery performance; safety; fast charging, power consumption of vehicles. The revolutionary strategy is targeting new vehicle power train systems which means developing the next generation of battery chemistries.

The roadmap for China is shown in Figure 24. In this figure, which is dated from 2015 to 2035 the Chines targets are compared to those of NEDO and the RISING program in Japan and with the Department of Energy (DOE) Battery 500 program. There are some discrepancies to what battery level we could reach in the future. [141]
India recently launched a roadmap for automotive manufacturing industries where batteries and battery production is described as highly strategic. Any targets for research to reach certain performances are not presented but clear statements on how important batteries are a key enabling technology are made [142].

Japan has a tradition of formulating long-term and stable research programs in certain key-areas. Batteries are one of them and the NEDO RISING-2 project which is a long-term large-scale initiative started 2010 and is planned to end 2022 [143]. It defines both the targets for battery performance (Figure 25) and the research efforts to reach the expected targets (Figure 26). This is the only international initiative where we see a clear comparison to the attempts we have suggesting the goals for BATTERY 2030+.
FIGURE 25 The Japanese and NEDO’s targets for battery performance 2020 and 2030.

FIGURE 26 The mission for battery research in Japan and the different targets and actions from 2010 to 2022.
US and DOE have also targets for the Battery 500 project which started 2016. Battery 500 is a collective effort with six universities, four national laboratories and IBM. It has the goal to develop lithium-metal batteries with almost triple the "specific energy" found in the batteries that power today's electric vehicles. The overall goal is to build a battery pack with a specific energy of 500 watt-hours per kilogram, compared to the 170-200 watt-hours per kilogram in today's typical electric vehicle battery. The Battery500 efforts will lead to smaller, lighter and less expensive electric vehicle batteries.

The research suggestions for BATTERY 2030+ are driven by identifying the roadblocks that need to be addressed to reach the goals of the SET-PLAN. It has thus a similar but far from identical approach as the Japanese RISING-2 projects. BATTERY 2030+ will also inspire a far larger community considering the research engagement in the different European member states and associated countries. In an international perspective we see the BATTERY 2030+ initiative as unique if it will be realized as a long-term effort.
7. References


[21] “EUDAT - Research Data Services, Expertise & Technology Solutions.”


[23] “UNICORE | Distributed computing and data resources.”


See e.g., “Wildcat Discovery Technologies.”

“Chemspeed.”

WWU Münster, “Developing future super-batteries.”


“ICSD - Inorganic Crystal Structure Database.”


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