European Commission

ROADMAP ON NEW AND EMERGING TECHNOLOGIES

Prepared by Working Group 1

#BatteriesEurope

Energy

Disclaimer
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List of Acronomys

AI	Artificial Intelligence
BIG	Battery Interface Genome
Br	Bromine
CEI	Cathode Electrolyte interface
EU	European Union
H2S	Hydrogen sulfide
IM	Insertion material
KPI	Key Performance Indicator
LCoE	Levelised Cost of Energy
Li	Lithium
LIB	Lithium-ion battery
MAP	Materials Acceleration Platform
Mn	Manganese
MWh	Megawatt hour
Na	Sodium
RFB	Redox Flow Battery
SEI	Solid Electrolyte Interface
SET Plan	Strategic Energy Technology Plan
TRL	Technology Readiness Level
VTOL	Vertical Take-off and Landing
Wh	Watt-hour
WiSE	Water in Salt Electrolyte
Zn	Zinc

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Executive Summary

This roadmap describes a long-term vision of the expected emerging and new battery technologies reaching as far as 2050.

The roadmap focuses on:

- Developing new battery chemistries and battery concepts (see Figure below) for a diverse range of present and future applications (Topic 1);
- Accelerating battery development and concept through the realization of new tools in the new area of digitalization (Topic 2).

Today, Lithium-ion batteries (LIBs) are a key enabler for decarbonisation of world

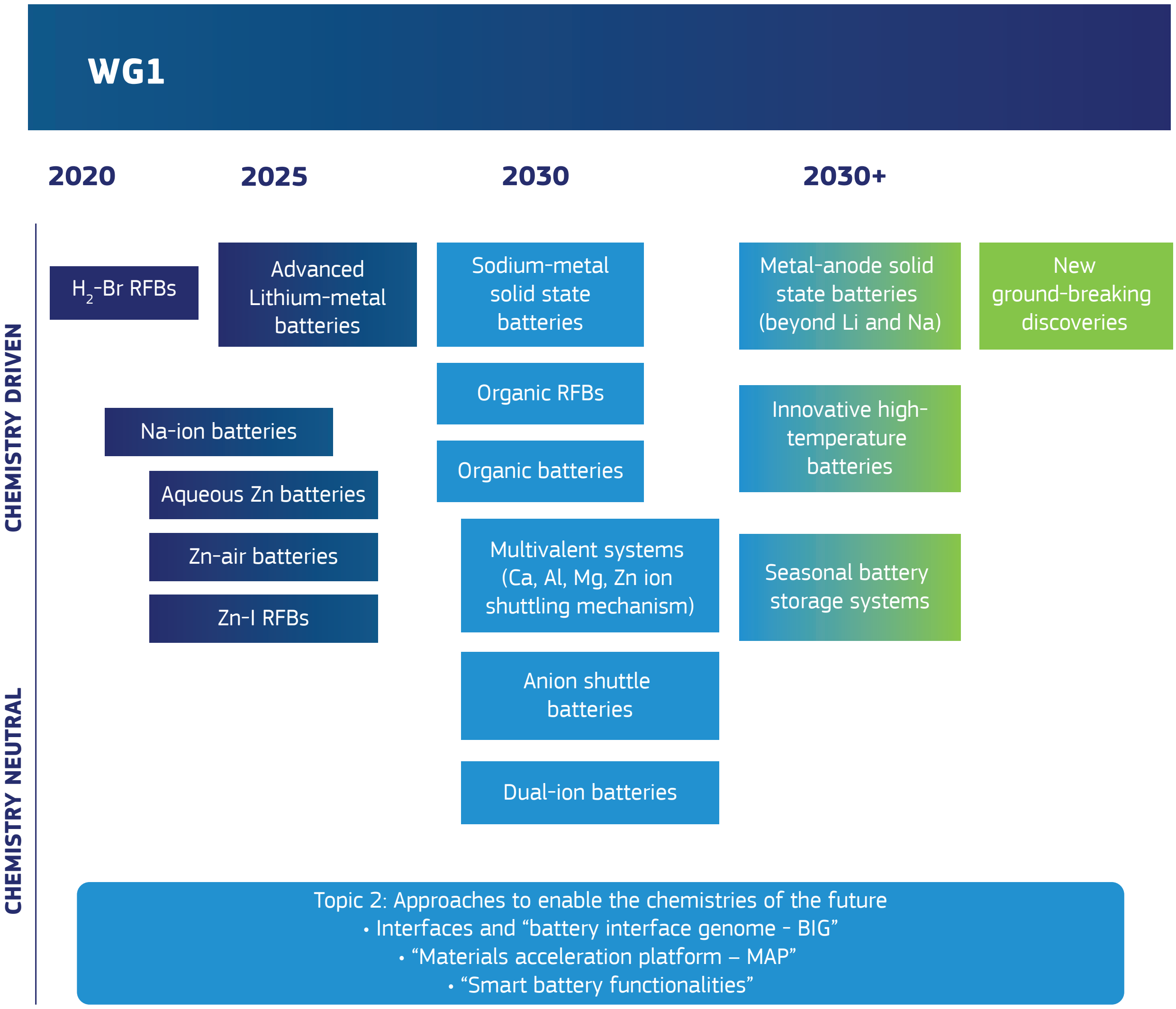


Figure A: Graphical representation of the new and emerging technologies roadmap developed by Batteries Europe WG1. The three time-points indicated (2025, 2030 and 2050) refer to when reliable, realistic and industrially relevant KPIs should be defined for the specific technologies. Such figure does not depict precise dates for market entry.

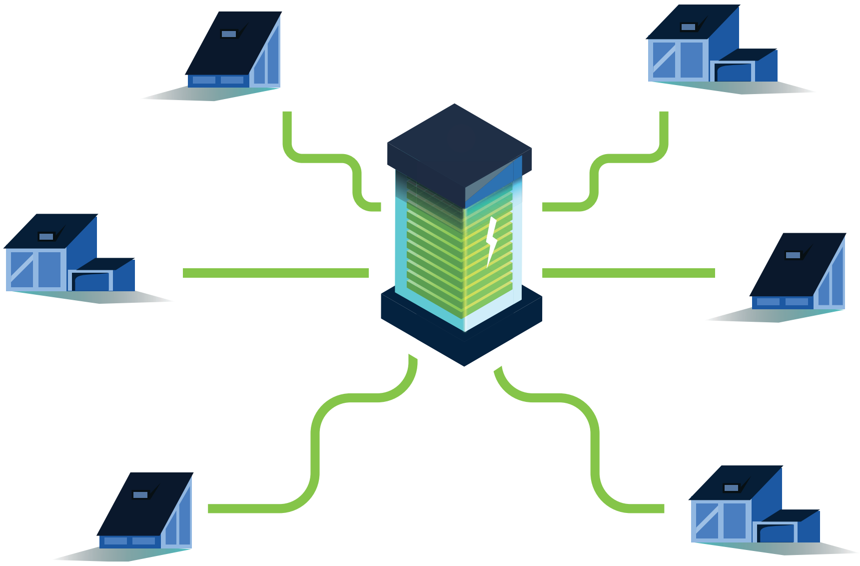
economy. At the same time, the energy transition will create new opportunities for a variety of different battery technologies to match safety, sustainability, circularity, cycle lifetime, performance, and cost requirements.
In order to reach these goals, it is recommended to:

1. Foster a pan European collaboration to accelerate the next battery chemistries by establishing infrastructure for enhanced cooperation.
2. Setup training programmes to help industry in their conversion to novel techniques and emerging technologies.
3. Stimulate long-term research to fully exploit new battery chemistries and enable ground-breaking discoveries.
4. Research networks to inspire and attract young bright minds and foster education at all levels.
5. Facilitate access to key infrastructures and small pre-pilot lines on an European level to accelerate development of new battery technologies.
6. Encourage with incentives industry to engage in early-stage research in order to promote technology transfer.
7. Specific resources to monitor the achievement of KPIs for new and emerging battery technologies, including actions toward:

    - Identifying new chemistries for existing and new applications;
    - Promote among scientists and facilitate patenting;
    - Identifying technologies ready for industrial development.

8. Encourage Member States to support basic research favouring international collaboration.

This roadmap is intended to provide guidance and suggestions on the next generation 1 cell technologies beyond the generation 3 and 4 of the SET-Plan[1].



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[1] See Appendix.

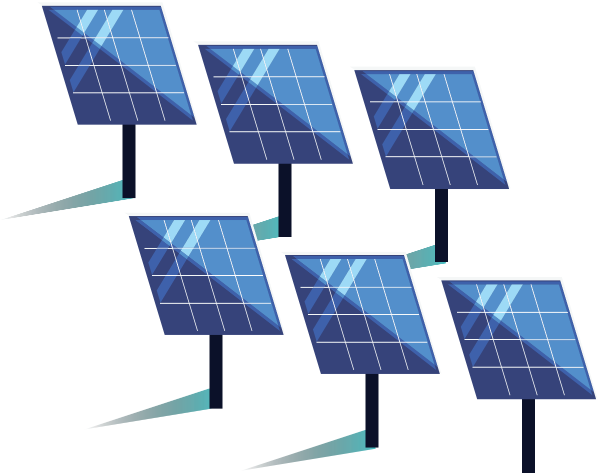
Vision

This roadmap comprises visions and expectations on future battery technologies and describes a long-term outlook, reaching as far as to 2050, which is the goal for Europe to reach a carbon neutral society, as stated in the Green Deal [2]. Future batteries should, in addition to terrestrial transportation, enable new applications such as Flying taxis (VTOL), Electric airplanes (commuter and hybrid planes), Domestic storage (day and night storage), Weekly storage and Seasonal storage. Also, tomorrow's medicine will generate new applications for external and implantable batteries, such as artificial muscles, hearing and sight support.

One of the keys to reach the targets of the Green deal is the development of new and emerging battery technologies with higher energy density at lower environmental footprints than today [2].

This is a broad view on possible battery chemistries that can be envisaged from 2025 and even longer-term. The roadmap describes the necessary means and measures to enable the future battery generations to enter the European battery market. The emerging batteries need to be produced, used, made "smarter" and recycled with a circular economic approach. Therefore, the focus is on future battery technologies, which are sustainable, long-lasting, low-cost, safe, and with high energy density.

This vision includes also tools to accelerate the innovation by developing new tools and to utilize the advances given by the new area of digitalization even including smart battery functionalities. The vision harmonizes to the needs for all future suggested battery chemistries to be addressed with clear views on recycling and manufacturability aspects.



Scope and objectives

The scope of this roadmap embraces both suggestions of future battery chemistries, battery technologies as well as tools and methods to reach the far fletching goals. It also identifies vectors for development of new and emerging technologies from fundamental understanding to practical applications.

Topic 1 deals with emerging technologies for which KPI-validation is expected to occur by 2030. It starts with generation 5 as stated in the SET-Plan [1] (limited to the transportation sector) but includes also battery technologies suitable for other sectors than transportation.

Topic 2 deals with approaches needed to accelerate the pace with which the new emerging battery technologies can be realised including also perspectives on manufacturability and recyclability. This topic is a summary of the comprehensive roadmap produced and developed within the BATTERY 2030+ framework.

New applications will require new battery technologies for which KPI validation is not foreseen within 2030. For some future technologies, the possibility to reach a level where KPI values can be defined are set to 2025 while more challenging technologies are expected to reach a level earliest by 2030.

The broader objective of this roadmap is to describe the challenges to enable new battery technologies, according to the SET-Plan, starting at generation 5 and beyond. In details, the objectives are:

- Pointing out the necessary directions to develop sustainable, safe, long-lasting and ultra-high-performance batteries;
- Developing a scenario which can give Europe a competitive edge in terms of new and emerging battery technologies considering availability of natural resources and sustainable approaches;
- Suggesting methods for accelerating the discovery and implementation of new battery storage chemistries and technologies;
- Developing smart functionalities in battery cells to enable very high life times which can be controlled in new battery management systems;
- Ensuring all new emerging technologies are recyclable and can be manufactured with climate-neutral approaches;
- Allowing for new unexpected discoveries encouraging Europe to support blue-sky risky research with the goal to provide European industry with innovative game-changing solutions on the long-term.

This Roadmap has been elaborated in

Methodology

a collaborative manner by the experts involved in Working Group 1 "New and Emerging technologies" of Batteries Europe, taking into account valuable comments and suggestions from Batteries Europe Governing Board and Secretariat, and EC officials.

The Batteries Europe WG1 management team including Chair, co-Chairs and Sherpa have worked together to generate a sound structure and preliminary draft of the document. Consultation workshops for all WG1 members were organized between January and March 2021. On a voluntarily basis, WG1 members were included into two groups, namely the writing and the feedback group with a total number of participants of around 25 members. Feedback, ideas and suggestions were collected from all participants during the workshops including the two groups. After the consultation, the management team incorporated and homogenised all contributes.

The document was finalised within a few on-line meetings and feedback given via a broad consultation of WG1 members, in addition to feedback from other Batteries Europe stakeholders.

1. STRATEGIC TOPIC 1: NEW AND EMERGING BATTERY CELLS

1.1 DESCRIPTION

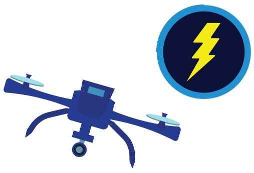
Almost thirty years after the first commercialisation of lithium-ion batteries (LIBs), the importance of the work conducted by, John B. Goodenough, M. Stanley Whittingham and Akira Yoshino, as well as the many other pioneering scientists around the world that contributed to this field was finally recognized with the Nobel prize in Chemistry in 2019 [3].

The success of this technology and the rapidly expanding market for energy storage, driven by automotive, but including also stationary and portable electronics applications, has recently raised concerns on the long-term availability of raw materials employed in LIBs, with projections predicting shortages in less than 5 years[2].

The increasingly growing need of LIBs and the consequent mass production have triggered attention toward the search for alternative battery technologies based on materials that can be sourced in a sustainable and responsible and employing non-critical raw material.

In 2018 the European Union proposed the ambitious vision to have a fossil-free society by 2050[3], gradually concretised through Green Deal measures. This is a strategic long-term vision plan toward a climate-neutral economy envisioning a complete transition to renewable sources. Achieving a carbon neutral society will require an electrification of most, if not all fossil fuel consuming technologies, putting even more demand on batteries.

New high-performance batteries will be needed for applications that are not fully matched by LIBs, such as vertical or short take-off and landing (VTOLs) and electric airplanes. There is therefore an urgent need to develop new chemistries and battery technologies that can be alternative solutions not necessarily competing with LIBs, in accordance with market diversification and different application requirements.



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[2] Lithium and cobalt – a tale of two commodities, McKinsey and Company, 2018.

[3] 2050 long term strategy "Clean planet for all" COM(2018) 773 final.

1.2 STATE OF THE ART

To have a clear understanding of the current state of the battery research, benchmarking and comparison of different battery technologies is fundamental. Work led and coordinated by Batteries Europe WG1 has involved a comprehensive overview of the state of the art of battery technologies. WG1 has identified and invited battery chemistry experts to review selected battery chemistries. Ten extensive reports on state-of–the-art battery technologies have been prepared and published in a special issue of the Journal of Power Sources in 2021[4]. They include contributions from a wide range of scientists from 50 institutes located in 12 EU and associated countries (see Appendix).

Herein, we discuss the state-of-the-art of battery technologies by considering the main challenges to be overcome for their main components.

1.2.1 METALLIC NEGATIVE ELECTRODES (ANODES)

Metallic negative electrodes have the potential to significantly increase the cell energy density since they are composed of the electroactive species only (e.g. lithium metal anode offers 10x capacity than graphite[5]). However, they all face two main challenges, i.e., unstable metal anode/electrolyte interfaces and interphases, and uneven metal deposition and stripping, both leading to poor performance and safety issues when flammable electrolytes are employed. The most promising approaches to tackle these challengesinvolve the use of solid electrolytes (possibly non-flammable or at least having low-voltility) and aqueous electrolytes.

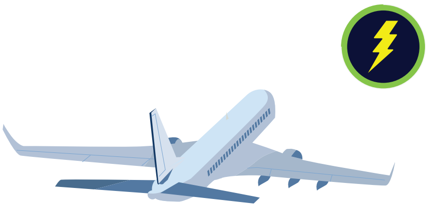
High-temperature, molten-metal batteries are another emerging technology intrinsically not affected by the two challenges mentioned above. However, their safety on large scale prototypes still needs to be greatly improved and subsequently demonstrated. Most of the activities performed so far involved modelling rather than experimental results [6].

1.2.2 ELECTROLYTES

In addition to higher safety, solid electrolytes can provide greater battery safety and may offer better electrochemical stability toward high voltage cathodes. In addition, cells can be assembled in bipolar series

connected configuration, reducing dead weight and volume. However, the only mature solid electrolyte technology involves solid state polymer electrolytes in Li metal batteries [7], which are susceptible to dendrites formation and have poor room temperature conductivities. Not restricted to lithium metal, sulphide solid electrolytes have much higher ionic conductivities, but are difficult to handle in air and can release highly toxic gases (Hydrogen Sulfide, H2S) if exposed to air and moisture. To maintain a good contact between the solid-state electrolyte and the electrodes, these cells need to be compressed, which adds extra weight to the battery. Ceramic electrolytes, in particular the NASICON electrolytes, offer the highest electrochemical stability window. They also possess very high hardness which may offer a good protection against dendrites, but they have lower conductivities and sodium dendrites have been shown to penetrate via the grain boundaries. For solid state electrolytes involving multivalent cations, further fundamental research is necessary to ensure charging rates are not significantly hindered that it would result in a less attractive product.

Aqueous electrolytes, including water-in-salt electrolytes (WiSE), strongly mitigate safety issues related to electrolyte flammability. They can also play an important role towards ecological, safer and less resource limited battery technologies such as zinc and sodium-ion batteries.



1.2.3 POSITIVE ELECTRODES (CATHODES) FOR POST-LITHIUM CHEMISTRIES

Lithium-ion[8] and lithium metal batteries [5] still offers the best prospects for high performance batteries, but new chemistries are starting to emerge which could alleviate the pressure on raw materials and hence have a lower cost base. However, positive electrodes for these emerging and new chemistries offering performance comparable or superior to the conventional Li-ion positive electrode insertion materials (IMs) need to be developed.

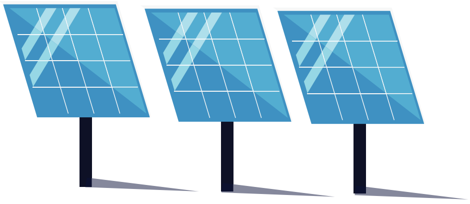
Sodium based batteries[9], and in particular sodium-ion batteries are among the emerging chemistries. These emerging cell technology making use of organic solvent- or aqueous zelectrolytes[10] can use existing Li-ion production lines and could reach energy densities close to current LIBs if high performance positive electrode materials can be identified. More disruptive sodium metal batteries are also being experimented with the prospects of high performance, high abundance materials and low cost, but they are at a very low TRL today.

Zn-IM cell technology employing Mn-based positive insertion materials (IM) and aqueous electrolytes are currently in an intermediate position between emerging and new technologies. Great progress has been achieved so far, making this cell technology one step closer to, but not reaching industrial readiness [11].

Conversion reaction-based positive electrode materials will be required to reach very high energy densities beyond today's stable cell configurations using traditional insertion materials.

Oxygen (from the air) or sulphur are interesting candidates as positive electrode active matter, but major breakthroughs are still needed. In this regard, electrically rechargeable Zn-air batteries are much more mature than their lithium counterpart although they still need substantial improvements before industrial upscale can be considered. Other new chemistries with much lower TRL's, but with much more abundant metals, include aluminium[12], calcium[13] magnesium[14] and zinc batteries[11].

Organic batteries are another class of early stage emerging batteries chemistry which do not use any metals as active material, but use the most abundant elements of the periodic table, carbon, nitrogen and oxygen. Nonetheless self-discharge, long term cycling stability, low density and calendar lifetime of the organic-based active materials need to be addressed. These organic batteries [15] are more advanced in redox-flow configuration because of their lower energy density. For these newer technologies, more basic science is needed to address the above mentioned issues.



1.2.4 REDOX FLOW BATTERIES (RFBS)

The Redox-Flow Battery (RFB) is not just another battery but a new class of electrochemical storage technology with almost infinite redox couple combinations possible[16] It is characterised by having all or part of the energy being stored separately from the power generator. Its lower energy density and very high cycle-life compared to "traditional" batteries makes RFBs more suitable for stationary applications today.

They can be divided into two categories:

those in which all the energy is stored outside of the power generator (e.g. vanadium RFBs), which gives total flexibility to size power and energy independently, and those in which part of the active material is stored in the generator (e.g. Zn-Br), sometimes called "hybrid" designs, which limits the maximum Energy/Power ratio. Vanadium and Zinc-Bromine redox flow batteries have now reached maturity and are being deployed for grid connected stationary storage at the 100's of MWh scale.

However, the use of vanadium will limit their cost reduction potential while the use of bromine has safety implications due to its toxicity. Hydrogen-Bromine RFBs are being demonstrated on the 100's kWh scale. They have the advantage of fast reaction, high power (1,4 W/cm^2) and high energy density (>200 Wh/L) but they also suffer from the risks associated with hydrogen (e.g. flammability, explosivity) and the toxicity of bromine. The Zinc-Iodine RFB has the same advantages as the Zinc-Bromine, but also has the safety advantage of a lower volatility.

New redox flow chemistries based on much more abundant and safer materials such as iron or organic and plant derived redox molecules offers new prospects for very low-cost energy storage, including decentralised long duration storage. The research possibilities in the molecular engineering of organic redox active matter are enormous and the field is very young. The main issues to solve are cycle and calendar stability, and energy density.

Most RFB designs rely on an ion conducting membrane to separate the positive and negative compartments. Very stable membranes such as perfluorinated polymers such as Nafion® are expensive and will limit the prospects for very low-cost storage once cheap and abundant active matter can be secured. Further research in anionic and cationic membranes, membrane-less designs and porous membrane designs will be necessary.

1.2.5 LONG TERM AND LONG DURATION STORAGE

Electricity storage within 4-12 hours (daily storage) is currently made possible with Li-ion technologies and upcoming Na-ion as well as redox flow batteries. Technologies that will enable "long-duration storage"[4] (more than 12 hours and up to one week of storage at nominal power), e.g. emerging redox flow batteries, and "long-term storage" (storage that can be used up to several

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[4] This broad topic is also present in the Working Group 6 (Stationary applications) roadmap. Working Group 1 considers low TRL at cell level and disruptive research towards new chemistries, and new cheaper materials to explore long term & long duration storage. Working Group 6 focuses on system level, current available chemistries aiming for high TRL, medium-to-long term & long duration storage.

months after charge, i.e. seasonal/annual) are of great interest.

Long-term storage technologies would enable the transfer of abundant solar energy in summer to be consumed in the low solar winter months. They could also help to level renewable energy consumption over one or two weeks and prevent incidents caused by a prolonged drop in renewable energy production caused by weather conditions, which would require more fossil fuelled plants to be used. Hydro is the main technology for this application, and it will be difficult to be competitive with this larger scale storage. Long term and long duration storage also imply a smaller number of cycles which automatically makes the LCoE or the cost per cycle more challenging for battery storage. However, pumped hydro has limitations in terms of geography and availability of suitable sites for new plants, and decentralised, smaller scale, long-duration or long-term storage could have a role to play if it can be made sufficiently cheap. Long-duration storage requires very cheap and abundant active materials to be competitive, for example bio sourced active matter. Long-term storage needs extremely low or zero self-discharge technologies. One solution would be to produce a high energy density and air stable material on charge which can be stored outside the battery, for example aluminium or zinc. This active matter can then be used several months later in a mechanically rechargeable battery, for example a metal-air battery. These are only examples, and other concepts may emerge if we are allowed to think outside the box.

1.3 WHAT IS NEEDED FOR EUROPE TO BE COMPETITIVE?

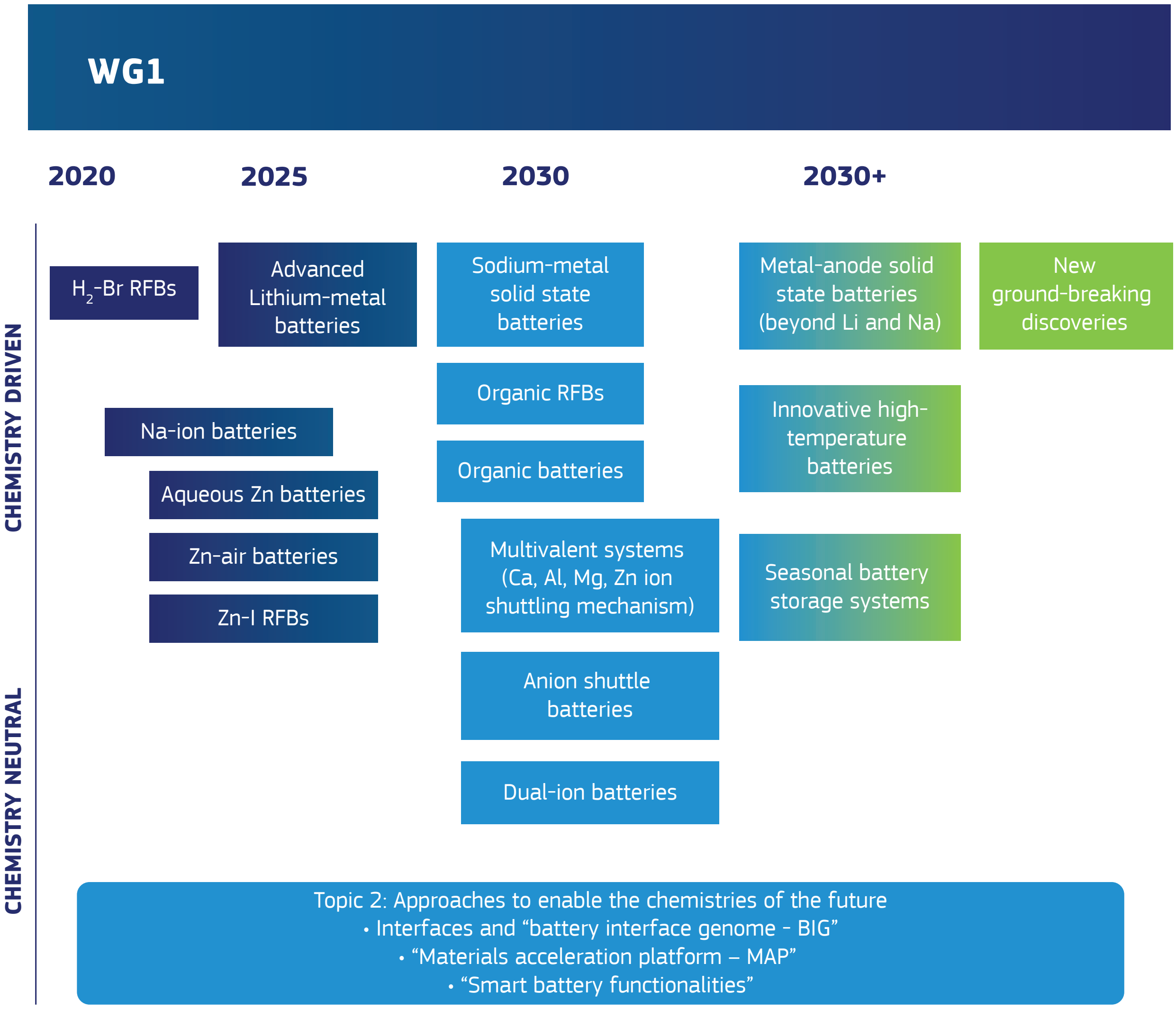
Europe can have a leading role in the development of green batteries by emphasising the environmental aspects of new and emerging technologies. These include, for example, green electrode processing, reducing the amount of organic solvents throughout the whole chain, use of aqueous electrolytes, batteries designed to be easily recyclable, use of abundant raw materials, batteries that favour second life applications. All these topics should be considered as central future research topics.

Access to key infrastructures and small pre-pilot lines on a European level by networking these high investment facilities would also help to accelerate development of new battery technologies. Pooling of resources for the creation of a “virtual” European Battery Institute, which could be delocalised in part in several countries, would also help Europe to be more competitive versus the American and Asian more unified approach.

1.4 RESEARCH NEEDS AND RESOURCES REQUIRED

To ensure competitiveness of new and emerging battery technologies with currently available options, focus should be placed on:

- Environmentally-friendliness (i.e., use of sustainable/circular materials);
- Low cost, easy access and sustainable extraction of raw materials;
- Sustainability and recyclability of entire system;
- Low-cost of the final battery technology;
- Low toxicity;
- High safety;
- Excellent performance metrics.



WG1

2020
2025
2030
2030+

CHEMISTRY DRIVEN
CHEMISTRY NEUTRAL

H_2-Br RFBs
Advanced Lithium-metal batteries
Sodium-metal solid state batteries
Metal-anode solid state batteries (beyond Li and Na)
New ground-breaking discoveries
Organic RFBs
Na-ion batteries
Innovative high-temperature batteries
Organic batteries
Aqueous Zn batteries
Zn-air batteries
Multivalent systems (Ca, Al, Mg, Zn ion shuttling mechanism)
Seasonal battery storage systems
Zn-I RFBs
Anion shuttle batteries
Dual-ion batteries

Topic 2: Approaches to enable the chemistries of the future
• Interfaces and “battery interface genome - BIG”
• “Materials acceleration platform – MAP”
• “Smart battery functionalities”

Figure A: Graphical representation of the new and emerging technologies roadmap developed by Batteries Europe WG1. The three time-points indicated (2025, 2030 and 2050) refer to when reliable, realistic and industrially relevant KPIs should be defined for the specific technologies. Such figure does not depict precise dates for market entry.

By considering the mentioned parameters, WG1 developed the graphical representation in Figure 1 identifying the most promising new and emerging technologies.

Assessing KPIs for new battery chemistries (beyond generation 5+) is a major challenge when benchmarking the progress of new and emerging technologies. The three time-points indicated in the graphical roadmap indicate three main targets summarized as:

- Short-term target (2025);
- Medium term target (2030);
- Long term target (2050).

The rationale behind this roadmap is that by 2025 and 2030 we should define reliable, realistic and industrially relevant KPIs for the specific technologies (see Fig. A), while in 2050 new cutting-edge research and ground-breaking discoveries are expected.

Resources needed to achieve WG1 targets (i.e., reliable KPIs definition- not technology development) are immediately necessary for all the above-mentioned chemistries (Fig. 1). In fact, once the definition of reliable KPIs for each battery chemistry is achieved, then the successful chemistries will be moved to higher TRL levels (industry development of materials and cells). Stable and long-term funding is foreseen for the continuous exploration of new battery chemistries originating from new cutting-edge research and ground-breaking discoveries.

2. STRATEGIC TOPIC 2: APPROACHES TO ENABLE THE BATTERIES OF THE FUTURE

The following topic and sub-topics are based on the BATTERY 2030+ roadmap [17] which is built on a chemistry neutral approach. This means that the actions suggested could be applied on any new and future emerging battery technology. All topics suggested needs also to take manufacturability and recyclability into account to ensure a circular economic approach.

Six research projects currently constitute the BATTERY 2030+ initiative[18].

The BIG-MAP project (coordinated by DTU in Denmark), focusses on Accelerated discovery of battery interfaces and materials. The INSTABAT project (coordinated by CEA France), SENSIBAT (coordinated by IKERLAN Spain), SPARTACUS (coordinated by Fraunhofer Germany), HIDDEN (coordinated by VTT Finland), and BAT4EVER (coordinated by VUB Belgium) work on self-healing technologies, contributing to the Integration of smart functionalities.

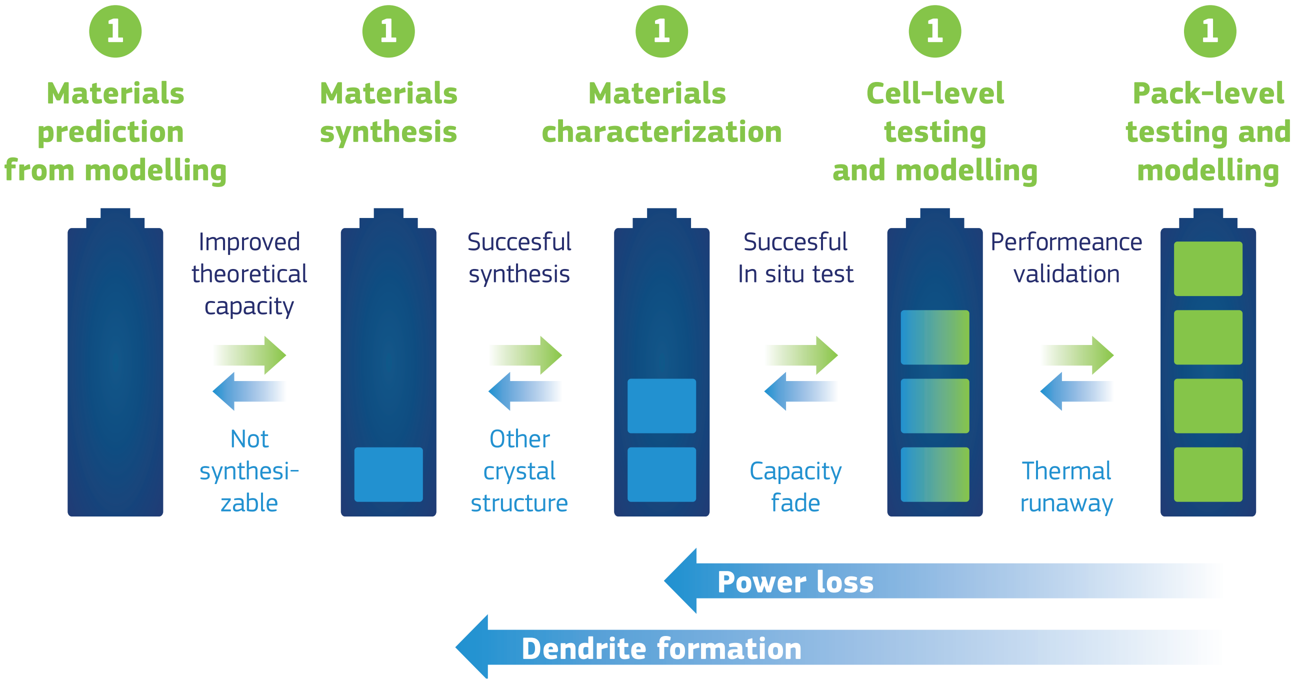
2.1 DESCRIPTION

Topic 2 is divided into three sub-topics that describe the most important roadblocks to handle for all possible new and emerging battery technologies: to understand reactions taking place at interfaces in battery cells that influence life-time, safety and the using of a possible chemistry; to accelerate the finding of new and emerging technologies utilizing digitalization and the rapid development of new theoretical tools in combination with the development of high-throughput experiments; and how to include new smart functionalities in a battery cell.

2.2 STATE OF THE ART

State-of-the-art in experimental and computational techniques for characterising battery materials and interfaces are targeting the scale of the atoms and ions. Conventional research strategies 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) (see Figure 2).

In recent years, a number of examples have emerged, where close an integration of virtual (typically



atomic-scale) computational materials design and operando characterization techniques in a circular design loop can accelerate the discovery cycle for next-generation battery technologies, e.g. high-capacity Li-ion cathodes and materials for secondary metal-air batteries, but further acceleration is needed to reach the highly ambitious goals formulated in the BATTERY 2030+ roadmap[17]. Ideally, such a circular materials development process results in a much more concurrent integration of experimental and theoretical research in an integrated development platform, which enables fast cross-fertilization of the results of complementary techniques.

Due to the complexity of interface formation, which is dynamic and dependent upon time-evolution, temperature, battery cycling conditions, as well as of the chemical matrix for the electrolytes consisting of different salts, additives and liquid solvents and/or solid components, there is still a lack of understanding hampering the engineering of new and emerging battery technologies. Going into more depth, at process level, the time- and the length-scale at which electrons are transferred remain almost completely underexplored. The experimental methodology needs to be further developed using the most advance synchrotron and neutron facilities, these advances going hand in hand with the modelling activities applying electronic structure and multi-scale modelling, as well as machine and deep learning to better extract the information from the data generated according to a battery interface genome – materials acceleration platform – BIG-MAP.

Even the best battery will eventually fail. Degenerative processes within a battery cannot be suppressed completely, and external factors such as extreme temperatures, mechanical stress, excessive power during operation, or simply ageing will in a given time act detrimentally on the battery performance. From the perspectives of sustainability and economic efficiency, particularly for critical applications, new ways need to be found to increase quality, safety, reliability and lifetime. This is today missing.

Here the three sub-topics are described.

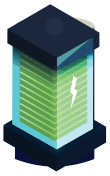
2.2.1 INTERFACES AND “BATTERY INTERFACE GENOME – BIG”

Interfaces in batteries are arguably the least understood part of any battery chemistry and assembly, despite the fact that most of the critical battery reactions occurs here, i.e. the charge transfer allowing shuttling Li or Na cations and electrons that trigger the formation of dendrites on lithium metal or sodium electrodes, the solid electrolyte interphase (SEI) formation and growth and the cathode electrolyte interface (CEI) that influence performance, safety and battery aging phenomena. Reliable and realistic methods for studying the formation and the continuous reactions during battery cycles need to be developed to go beyond our current understanding that is largely limited to post mortem studies.

Almost all different battery chemistry technologies proposed need to control, engineer and modify interfaces on battery electrode materials, as well as between the different components in the battery.

Two parts are necessary: the development of high-throughput operando techniques for interface and electron monitoring and the accelerated characterization, prediction and design of battery interfaces, the so-called “Battery Interface/Interphase Genome” (BIG)[18], by the combination of deep learning, multi-scale modelling and high-throughput experiments and testing.

2.2.2 “MATERIALS ACCELERATION PLATFORM – MAP”



There is an urgent need to accelerate the exploration of new battery materials, electrolytes and interfaces/interphases, by implementation of a Materials Acceleration Platform (MAP) [18]. The MAP will enable closed-loop discovery and development materials and cells through the use of Artificial Intelligence (AI) to orchestrate multi-sourced 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 utilizing the Europe large-scale synchrotron and neutron facilities, as well as EuroHPC infrastructure for the modelling and data analysis.

The MAP infrastructure should be modular and highly versatile, in order to accommodate all emerging battery chemistries, material compositions, structures, and interfaces. MAP utilises AI to integrate and orchestrate data acquisition and utilisation from a number of complementary approaches and technologies. The expected impact is up to 5-10-fold increase in the rate of discovery of novel materials and interfaces.

2.2.3 “SMART BATTERY FUNCTIONALITIES”

Smart battery functionalities which is a field of the high potential of innovation evolving from new ideas how to improve safety, quality and reliability on the cell level. At this stage it is based on miniaturized advanced sensors, build in directly into battery cells with ability to detect dysfunctional components of the battery cell with spatial and time resolutions, and thus probe reactions occurring at interfaces (Currently running projects: INSTABAT, SENSIBAT, SPARTACUS,BAT4EVER, and HIDDEN) [18]. It also describes a relatively new and unexplored area for batteries based on self-healing functionalities. Inspired by the field of drug delivery and of the paint industry where these concepts have developed, autonomous and on demand self-healing functionalities can be made to increase the life time of a battery cell.

All new disruptive ideas tested with sensing and self-healing chemistries must be upscale, manufactured and recycled simply and in an affordable manner.

2.3 WHAT IS NEEDED FOR EUROPE TO BE COMPETITIVE?

EU needs to support building up a tool-box to accelerate the discovery of components and cell designs of new and emerging battery technologies (topic 1 in this roadmap). For all future battery chemistries to be realistic alternatives for future applications, and for European industry to become long-term competitive, we need to control and understand, and ultimately predict and prevent unwanted side reactions at the interfaces between the different components in a battery.

To accelerate the discovery and development of new materials and battery concepts which will in turn increase the competitiveness of the battery industry in Europe, the full utilization of the rapid advancement in digitalized tools, such as AI/machine learning and autonomous synthesis robotics, is essential. The data generated across different length and time scales using a wide range of complementary approaches, including computer simulations, autonomous high-throughput material syntheses and characterisation, in-operando experiments, and device-level testing, will all contribute to the development of new material and battery cells.

'Smart functionalities' are the key to next-generation technologies and that have been rarely explored concept on the field of battery cells. This will enable the realisation of safer, reliable and more durable battery chemistries. It is a holy grail of multi-disciplinary design. It may be the effort that allows European battery research to leapfrog to the highest international level.

2.4 RESEARCH NEEDS AND RESOURCES REQUIRED

The research efforts and the resources required for topic 2 is almost a limitless assignment with the need to merge data, soft/hardware infrastructures from all relevant scientific and innovation communities along the entire battery value chain to make true progress.

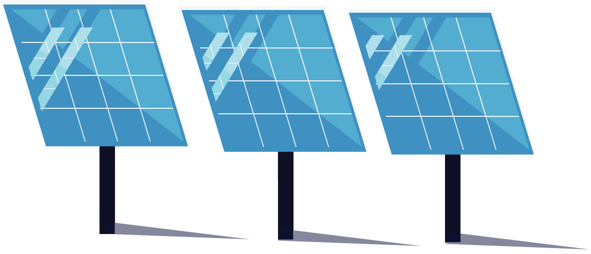
We have therefore summarised the most important points here:

Pushing the frontiers of in situ analytical characterisation techniques to direct realistic operando techniques is a considerable challenge but also a must for the development of the future sustainable battery chemistries.

- EU needs to the access and support the development of analytical techniques that would allow to realistically follow the movement of interfacial reactions at the molecular scale all the way to the role of electrons at the nanoscale and sub-nanoscale, at relevant timescales and on relevant systems and interfaces.

To accelerate the discovery and development of new materials and battery concepts to increase the competitiveness the battery industry in Europe:

- EU needs to support the development of digitalized tools in combination with high-throughput experiments in a closed-loop discovery process. This needs to be rapidly developed



to common experimental and testing protocols and a shared community-wide European infrastructure for performing, storing and sharing data, i.e. the autonomous acquisition, handling, and analysis of data from all domains of the battery development cycle.

Batteries are operating in different conditions, curative functionalities which would enable battery operation in different non-ideal conditions needs to be developed, such as: smart functionalities with sensing developed to detect irreversible reactions and self-healing functionalities designed to repair damage occurred within the cell.

- The EU needs to establish a new research community including a wide range of R&D disciplines to enable sensor and self-healing functionalities.

The needs are expressed with a longer-than-ten-year horizon; needless to say, realizing this long-term vision requires several research facets with their own fundamental challenges and technological bottlenecks.

3. PRIORITISATIONS & KEY RECOMMENDATIONS

Ample resources are needed to merge topic 1 and topic 2 into a holistic approach to enable the batteries of the future, and we need to start now for the sake of Europe's battery industry.

Priority should be given to those technologies for which KPIs can be addressed/identified sooner to enable Europe to gain the competitive edge in the production of emerging battery technologies. Digital platforms for accelerated materials discovery, high throughput experiments, and smart battery functionalities will be significant catalysts for the development of these emerging technologies.

Nonetheless, blue sky research must be also supported in this field to inspire breakthrough ideas and concepts for game changing technologies.

Key recommendations:

- Foster a pan European collaboration to accelerate the next battery chemistries by establishing infrastructure for enhanced cooperation;
- Training programme to help industry in the conversion to novel techniques and emerging technologies;
- Long-term research for full exploitation of new battery chemistries and ground-breaking discoveries;
- Research networks to inspire and attract young bright minds and foster education at all levels;
- Encouraging with incentives industry to engage in early-stage research in order to promote technology transfer;
- Providing specific resources to monitor the achievement of KPIs for new and emerging battery technologies, including actions toward:
    - Identifying new chemistries toward existing and new applications;
    - Promoting and facilitating patenting among scientists;
    - Identifying technologies ready for industrial development;
    - Encouraging Member States to support basic research favouring international collaboration.

4. CONCLUSIONS

The EU is accelerating LIB production, but has the opportunity to be a key player in the development of new and emerging battery technologies.

To attain this goal the EU needs to:

- Develop batteries that can be competitively produced according to the high Europe an environmental and safety standards (upcoming Batteries regulation). This requires the use of sustainable, cheap, non-polluting materials and processes;
- Leverage on existing national research and industrial capabilities to create a unified pan European landscape in order to match the concerted efforts put in place in the other large economies in the world;
- Foster innovative educational initiatives including cross-over of academia and industry to prepare highly qualified and skilled workers.

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Appendix

Table 1: Li-ion batteries Generations

Generation	1	2		3		4			5
		2a	2b	3a	3b	4a	4b	4c	
Type	Current	Current	State-of-The-Art	Advanced Lion HC	Advanced Lion HC	Solid State			Beyond Li-ion
Expected Commercialisation	Commercialised	Commercialised		2020	2025	>2025			
Cathode	NMC/NCA LFP LMO	NMC111	NMC424 NMC523	NMC622 NMC811	HE NMC Li-rich NMC HVS	NMC	NMC	HE NMC	
Anode	Modifed Gaphite $Li_4Ti_5O_{12}$	Modified Graphite	Modified Graphite	NMC910 Carbon (Graphite)+Si	Silicon/Carbon (C/Si)	Silicon/Carbon (C/Si)	Li metal		Li metal
Electrolyte	Organic LiPF6salts			(5-10%)	Organic+ Additives	Solid electrolyte -Polymer (+Additives) -Inogranic -Hybrid			
Separator	Porous Polymer Membranes								

Source: Nationale Plattform Elektromobilität, Marcel Meeus, JRC.

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