European Commission

# ROADMAP ON CELL DESIGN AND MANUFACTURING

**Prepared by Working Group 4**

#BatteriesEurope

Energy

Disclaimer

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# Acknowledgements

The presented roadmap is the combined effort of long discussions, brainstorming sessions and work load put in by the members of the WG4. Without their commitment and hard work, this roadmap document would not have been possible. Collecting the information and combining all the discussion topics has been a tremendous effort and shall form the basis for the future development program, which also affects the rest of the battery development value chain. Special gratitude is expressed to the Chairs, Sherpa and co-Chairs of WG4, who have led the discussions and made the often difficult decisions to cut and condense the very extensive content created by the team towards a concise and presentable roadmap. The focused roadmap will guide the R&D strategy of the EU within the area of cell design and manufacturing.

# List of Acronomys

| | |
|---|---|
| **AI** | Artificial Intelligence |
| **CAPEX** | Capital Expenditure |
| **ETIP** | European Technology & Innovation Platform |
| **KPI** | Key performance indicator |
| **ML** | Machine Learning |
| **Ni-MH** | Nickel–Metal Hydride |
| **NMP** | N-methylpyrrolidinone |
| **OPEX** | Operational Expenditure |
| **R&D** | Research and Development |
| **R&I** | Research and Innovation |
| **s-LCA** | Social Life Cycle Assessment |
| **WG** | Working Group |

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# Executive Summary

The European battery cell manufacturing industry, as a strategic sector for the European economy, aims to become the world leader on sustainable and innovative battery cell production, while supporting the electrification of transport globally and providing stationary energy storage solutions to support the transition to renewable energy sources.

The complexity of the battery cell and its production process requires an interdisciplinary approach in which European core competencies need to be bundled and extended to promote a successful battery production. Creating a qualified local vertical supply chain is essential for the European ecosystem, and to achieve this goal, developments in processing technology, equipment design, manufacturing, and digitalization all through the manufacturing value chain is needed to implement the already highly innovative material development into industrial realisation. Several initiatives have been created to support this R&I ecosystem across Europe, with Battery2030+ and LiPlanet being two outstanding examples.

European-made batteries aim not only to achieve better performance -higher energy density, fast charging capability-, but also to be safe, affordable and the most innovative and sustainable. Innovative cell components and design as well as manufacturing processes and machinery are fundamental to a continuously improving battery cell performance while simultaneously reducing costs and environmental impact. Environmentally friendly production of cell components (e.g. water-based or solvent-free coatings) is crucial. In addition, a knowledge-based product development and production process must be promoted in order to avoid expensive trial-and-error operation. This is valid both for current state-of-the-art battery technologies up to Generation 3[1] as well as for upcoming solid electrolyte battery technologies -Generation 4- and to anticipate manufacturing needs and solutions for future battery technologies to come -Generation 5-.

For Europe to be fully successful, the entire life cycle must be included in the product design and the production process to foster a circular economy in which battery cells can be recycled at their end-of-life and the overall environmental impact is reduced to a minimum. In order to produce high-performance batteries with high efficiency, there is a need to develop and utilise models that can predict (on the basis of experimental data and rapid parameterisation methods) the

[1] See Appendix.

compositions of the various battery components that will provide the best energy densities and the lowest costs. Here, all processes associated with the entire life cycle could be verified and criteria for recyclability and social impact included in the design phase of a battery.

As a consequence, digitalization emerges as a new paradigm that will certainly be applied at several levels within the battery industry. Digitalization is a decisive enabler not only to uncover cause-effect relations within the battery cell and along the design and production line, but also to enable fully automated production lines resulting in higher battery cell performances, quality control and production yields. Better quality can be ensured through the implementation of the battery passport concept[2] and digital twinning of manufacturing and battery management through sensors, automation and AI process controls, and ultimately leads to competitive battery performance and cost.

Production lines must be flexible against the background of ever-changing cell formats and production technologies (e.g. upcoming of extrusion-based mixing, dry-coating, continuous cell assembly). Here the definition of machine standards for control technology should be purposeful. Digital twins should be used to reduce production bottlenecks and design errors. In addition, artificial intelligence and machine learning need to be used in the future to accelerate the development of new processes and equipment. In addition, new factories must be integrated in local ecosystems in order to increase the overall efficiency of the factory and simultaneously decrease environmental impact to a minimum – this includes both access to renewable energy sources as well as the customer market.

This roadmap is focused on the Li ion battery technologies, as the mastering of lithium ion and related battery generations is what will make the difference for Europe to be successful in the rapidly expanding battery market.
The core of the development focus within Cell Design and Manufacturing for meeting industrial needs has been identified as:

- Reducing the total battery manufacturing cost which is a key task while keeping sustainability at the core;
- The efficient design of cells and its components to increase cell energy density and fast charging capability while maintaining and potentially improving safety levels;
- Incorporation of recyclability and social impact criteria into the design phase of a battery;
- A transformation into digitalized processes as the key to unlock optimization potential across the battery value chain.

[2] https://ec.europa.eu/commission/presscorner/detail/en/qanda_20_2311.

# Vision

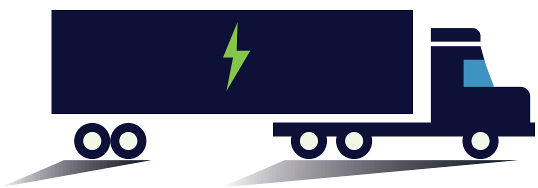
For Europe to be successful in its goals to reach zero emissions by 2050, the advancement and integration of battery technology for both the transport and stationary energy storage will be a key enabler. It is essential to further develop and build on Europe's strengths all along the battery value chain and to further develop in particularly battery cell manufacturing technology. Strong capabilities in materials development, digitalisation and applications engineering are the necessary foundation of sustainable and innovative battery cell manufacturing in Europe. In recent years, most European R&I efforts have focused on developing new battery technologies, materials, applications and others- with insufficient efforts specifically focused in cell design and manufacturing.

Europe currently has a great opportunity for implementing more sustainability and innovative manufacturing processes with the establishment of giga-scale battery production. To achieve these targets, this Roadmap proposes an R&I strategy focusing on two strategic areas:

The first line of action focuses on technology and equipment development, addressing new production methodologies for current and new chemistries, minimizing costs and environmental impact, including recycling efforts and sustainable production.

The second area is utilising digitalization, a key horizontal approach addressing developments from the cell design, to equipment and production line digital twinning, up to plant site local ecosystem optimization. Digitalization not only will shorten development times, but also will bring quality and efficiency in production to the next level.

The time scale for realising this vision and the steps necessary to be taken are outlined in this document as well as highlighted in Figure A.



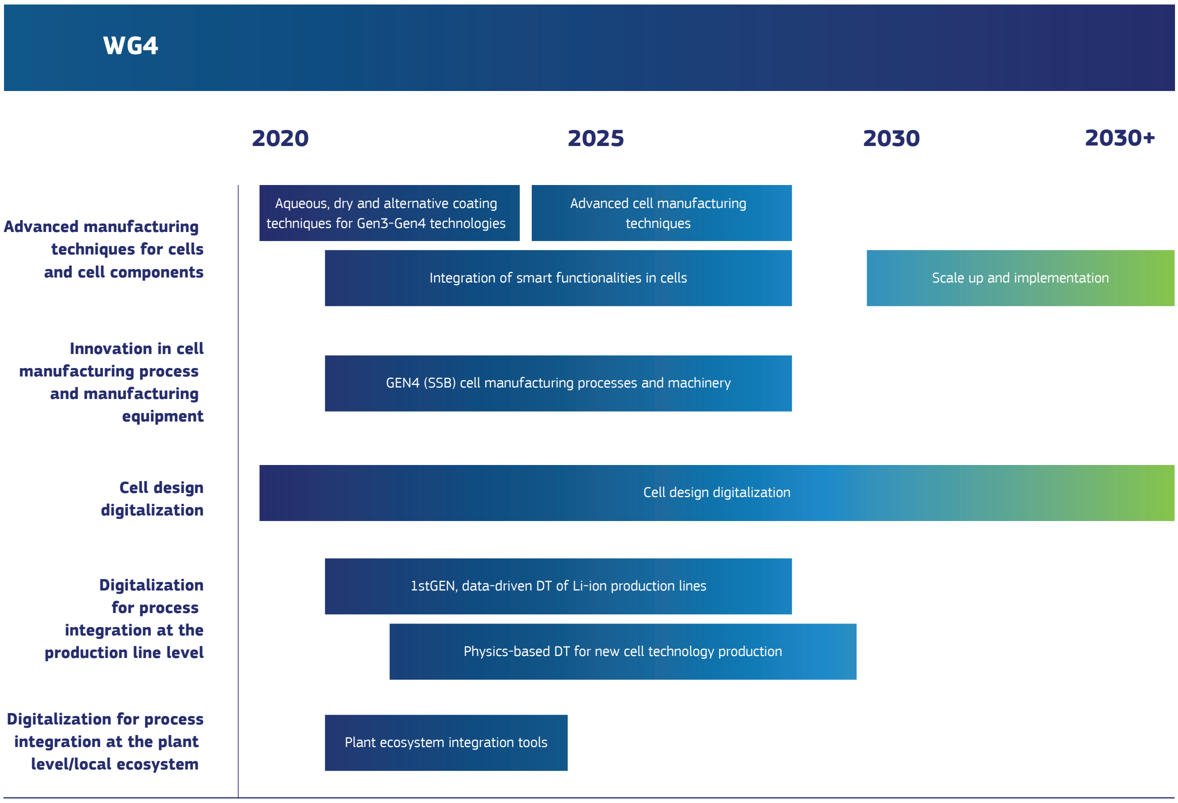
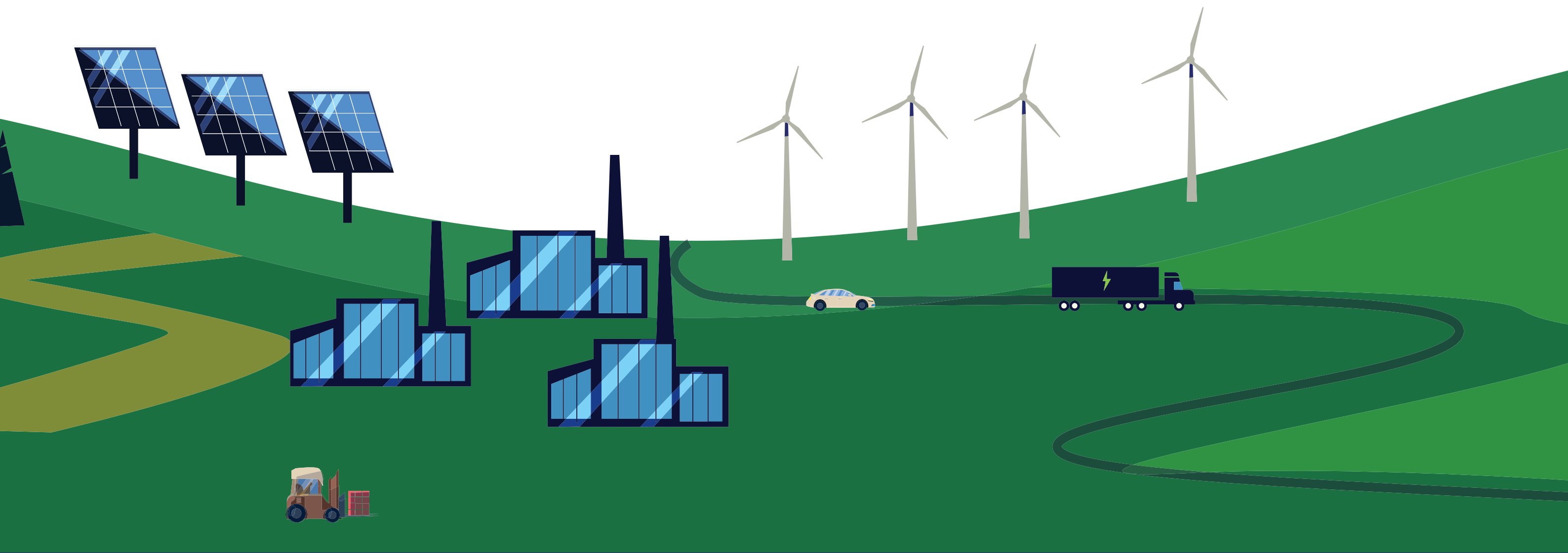



Figure A: Graphical representation of the strategic topics for cell design and manufacturing in the period 2020-2030+, developed by Batteries Europe Working Group 4



# Scope and Objectives

Europe aims to become the second largest battery producing region worldwide by 2025[3]. To meet this ambitious goal, it is mandatory to create a qualified local vertical supply chain.

Continuous improvement driven by the growing demands towards batteries in various application fields are supported in part by technology and material evolution and in part by battery design modifications. These evolutions will require fast reaction and implementation. A close cooperation between processing technology developers, machine providers and battery makers is required. Thousands of qualified technologist, engineers and technicians are needed, who will have to support multiple production factories on a GWh scales in a relatively short period.

This approach is necessary but not sufficient to make the EU battery competitive. Improvement and innovation in the state-of-the-art cell design, cell components, manufacturing equipment and process as well as a closed material loop are also required to ensure competitiveness in the long term. Furthermore, as cell technologies continue to evolve and adapt to specific applications or materials, production equipment design must follow (or even anticipate) those trends to ensure a smooth transition between the design phase and industrialization.

Reducing the total battery manufacturing cost is a key task while keeping sustainability at its core. For the European industry to succeed, cell design and manufacturing technologies have to support the industrial production to improve its key performance indicators (KPIs) while reducing global environmental impact. In Annex I, table 1, several KPIs for the current generation of Li-ion batteries and for 2030 scenarios are presented. Further actions will be required to better define those KPIs.

Although it is recognised that several battery technologies coexist in the state-of-the-art -including "classical" such as lead acid or Ni-MH, or alternative approaches like redox flow batteries, it is widely accepted that the dominating technology that remains at the core of the electrification revolution is lithium ion and its different evolutions.

Therefore, focusing the actions proposed in this Roadmap into the different generations of lithium-ion battery technologies will maximize impact and resources utilisation. Having recognised the contribution of battery technologies other than the lithium-

[3] European Battery Alliance (reviewed 08/2021)

ion family, they may well be included in future revisions of this roadmap as the market evolution will call for them.

Specific R&D initiatives are needed to help establish a powerful research network and battery industry within Europe that is able to develop and establish new and innovative technologies along the battery value chain. KPIs will serve as a reference baseline to evaluate those initiatives and ensure that the new technologies are competitive.

In the following chapters, R&D actions are further described, focusing on two main directions:

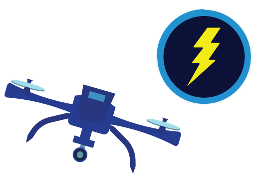
1. Manufacturing technology, equipment development and sustainability.
2. Implementing Digitalization through all the value chain.

New manufacturing process for current generation battery cells (i.e. raw-to-powder process, fast assembly and predictive formation) and suggestion on cell design and components are presented. Moreover, the recyclability of cells (design for recycling) as well as, their potential use in second life applications will become more and more important

Digitalization, both at production and plant level, is a necessary element for the battery industry to make progress towards a fully aligned and competitive industry 4.0 ecosystem. Different tools are described in the specific section, from digital twins to sensors.

R&D actions will focus on short and medium term, 5 to 10 years, where specific improvements on current generation technologies are required. Long term actions (2030-2050) are also presented, all of them in coherence with developments under BATTERY2030+ Initiative.

This roadmap focuses on R&I needs that are identified by academia and industry and cannot fully represent the industrial presence of all parts of the battery manufacturing value chain. For instance, Li metal foil supply within Europe is not only a matter of R&I, but rather a lack of European businesses within this sector – therefore it will not be covered within this roadmap, although it is needed to enable advanced R&I actions, especially for generation 4 production technologies.



# Methodology

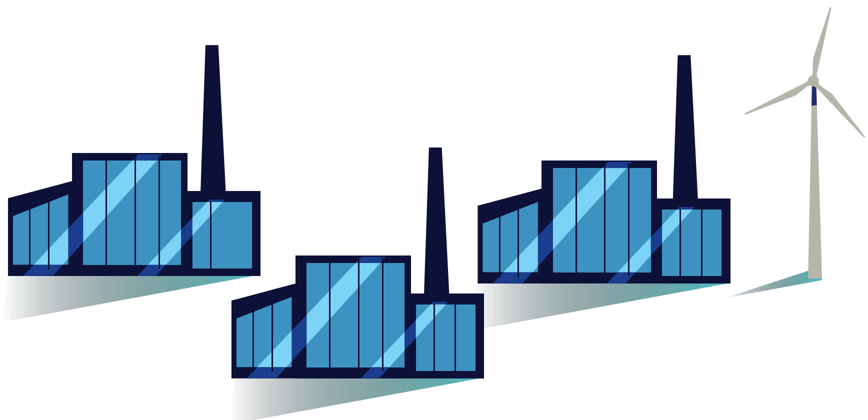
This Roadmap has been elaborated in a collaborative manner within the experts involved in Working Group 4 "WG4: Battery Cell Design and Manufacturing" of ETIP Batteries Europe, plus additional valuable comments and suggestions from Batteries Europe Governing Board and Secretary, and EC officials.

The natural starting point was taken at the Strategic Research Agenda released by Batteries Europe on 4/12/2020, organised in several chapters dealing with specific parts of the batteries value chain. The section on battery cell design and manufacturing, also drafted and prioritised by WG4, already outlined four strategic topics, the last one grouping two related, but identifiable as stand-alone topics. This package of up to five strategic topics were further elaborated and developed within WG4, giving shape to this Roadmap.

A kick-off meeting was held on 10/12/2020 involving the whole WG4, where the first approach to this roadmap, as prepared by the WG4 Management Team -composed of Chair, Sherpa and co-Chairs- was presented and validated. Volunteers were identified to join the writing team. After several iterations and many teleconference discussions over Q1/2021 the present Roadmap structure was developed, where the original five strategic topics depicted in the SRA were grouped into two larger, umbrella strategic topics for the shake of clarity. More than 25 experts were involved at this point in drafting the roadmap.

A final Roadmap WG4 General Assembly was held on at the end of March 2021 to validate the first full draft of this Roadmap and to provide additional comments and improvements. After this point, the feedback and guidance from Batteries Europe Governing Board, Secretariat and EC officials has been instrumental in giving it its final shape.

The WG4 Management Team greatly acknowledges the contributions to this Roadmap to all the parties involved.



# 1. STRATEGIC TOPIC 1: TECHNOLOGY GENERATION - BATTERY CELL MANUFACTURING TECHNIQUES, PROCESSES AND EQUIPMENT

## 1.1 CELL COMPONENTS & DESIGN

For the EU Battery manufacturing industry to be competitive a qualified local supply chain is necessary, including the development of batteries with improved performance and safety at reduced cost. The state-of-the-art in the battery sector evolves at a rapid pace with an increasingly fast availability of new advanced materials and components with improved performance. Continuous improvement driven in part by battery design modification will require fast reaction and implementation. This will be possible if close cooperation between machines supplier and battery makers is established.

This approach is necessary but not sufficient to make the EU battery industry grow stronger. Improvement and innovation in the state-of-the-art battery cell components, cell design, manufacturing equipment and process are also required to ensure competitiveness in the long term and total environmental impact reduction. Additional effort needs to be made in real-time monitoring and self-learning manufacturing processes, in optimizing energy intensive processes and material usage effectiveness. The design for intrinsic safety and recycling should be considered at the conception phase of the cells.

### 1.1.1 STATE OF THE ART

Due to the multitude of components that are contained in a lithium-ion battery cell, as well as a number of production concepts that define the cells, there is a wide variety of cells designs. Three different forms are used: cylindrical, prismatic or pouch cells. In all cases, the main components of the cell are essentially the same: electrodes made of a mixture of active material, binder and conductive additives deposited on thin current collectors made of Al or Cu, a separator, a liquid electrolyte and a casing, either metallic -rigid- or multilayer -flexible.

Electrode manufacturing processes today are mostly based on continuous wet coating of active material mixtures ("slurries") on top of the current collectors. These are composed of >90% active material, plus several additives including carbon components as conductivity enhancers, and polymers as binders to ensure cohesion and adherence to the substrate. Such wet coating is traditionally done by dispersing the solid content in an organic media such as N-methylpyrrolidinone (NMP) solvent. Recently there has been a shift towards using water instead of organic solvents, especially for anodes, requiring different processing conditions and slurry composition -e.g., hydrocarbon-based binders instead of fluoropolymers. Typically, water processing of cathode active materials is more challenging due to the risk of leaching metal cation components into the dispersing media.

## 1.1.2 R&I NEEDS

- Increase energy density through cell and component design;
- Increase safety by cell casing, component selection and cell level sensing and smart cell design;
- Environmentally friendly manufacturing of cell components, including coatings (e.g. water based or solvent free coatings);
- Solid electrolyte architecture design for optimised dendrite protection and high voltage operation;
- interface phenomena between components of all-solid-state batteries (Generation 4);
- maximum charge / discharge rate capability of high energy cells via electrode design, e.g. via electrode structuring;
- and facilitate access to reproducible Li foil and Li coated foils to further develop its use and protection.

## 1.2 PROCESS AND EQUIPMENT DEVELOPMENT

In the next 5 to 10 years period the focus should be in introducing new manufacturing process for current generation battery cells and modules (i.e. raw materials-to-powder process, fast assembly and predictive formation) to increase their production yield and efficiency while reducing the total CAPEX and OPEX. Increasing safety through smart cell design and cell specific safety measures will also be necessary.

In parallel, highly automated processes need to be developed and deployed at pilot scale to enable next-generation technologies production, including all solid-state and metal electrodes based / metal air battery cells and modules.

## 1.2.1 STATE OF THE ART

State-of-the-art processes and equipment for current generation battery cells are still based on the concepts developed by the Japanese battery industry in the 90's. Manufacturing processes consist of wet electrode preparation and drying followed by assembly in a complete cell which is electrochemically formed and aged. The overall process is energy-intensive and there are numerous potentials processes in which efficiency may be improved.

New trends in battery cell technologies such as the introduction of solid or semi-solid electrolytes, as well as lithium metal sheets as anodes -as in Generation 4 batteries-, are challenging the established state of the art on electrode and cell manufacturing, as well as the equipment used for handling and cell assembly. Also, no specific automation is available as the final product and manufacturing process are still in a R&D phase. Conventional electrode fabrication processes as described above are therefore limited when they are confronted with these new approaches.

Also, there is ample room for improvement and optimization of the current graphite anode and liquid electrolyte cell technologies (Generation 3) via the introduction of a gradient of tri-dimensional textures through the electrode active layer, micropatterning of the electrode surface or other concepts. All these are difficult if not impossible to implement with the current electrode manufacturing techniques and technologies.

## 1.2.2 R&I NEEDS

- Green manufacturing of cell components, including coatings (e.g. water based or solvent free coatings);
- Advanced equipment for electrode production, including dry mixing and casting technology to reduce the solvent required and increment the production yield;
- Increasing the yield while reducing the environmental impact (both in terms of emission and waste production) and energy efficiency / consumption are key targets for the European industry;
- Implementation of Generation 4 architectures, especially solid electrolytes, including establishing manufacturing processes;
- and equipment retrofit to adopt to Generation 4 technology where possible;
- and/or predictive formation algorithm to reduce the CAPEX and

OPEX impact in the manufacturing equipment;

- New production process in the medium term, such as powder-to-roll electrode preparation (dry production and solvent involved), flexible high-speed assembly process of different formats (pouch, cylindrical and prismatic) and sizes (including high energy large format cells by using the same machinery with different tools to produce different cell stack sizes) and new approach for the formation process to reduce their duration;
- Implementation of new manufacturing processes and equipment as by innovative cell and module design with intrinsic safety and sensor in cell embedding;
- Manufacturing of electrodes and cells with Generation 4 materials with minimal needs for adapting assembly technologies;
- Increase manufacturing yield, e.g. by real-time in-line inspection methods.

## 1.3 RECYCLING AND SUSTAINABILITY

The goal of achieving a leading position in battery manufacturing also includes the lead in sustainability and the use of innovative materials and processes. In fact, it might be the largest differentiating factor for the European battery industry. There are great opportunities in using renewable energies for cell factories, increase the use of recycled materials within the cells, modules and packs as well as completing the value chain with a circular economy approach throughout.

### 1.3.1 STATE OF THE ART

In the manufacturing processes there are several areas where a focus on lowering the energy demand and improving recyclability can be addressed. Today's aqueous coating is regarded as more environmentally friendly than coating with organic based slurries, as it does not involve volatile organic compounds emissions. However, wet coating limits the processing speed to make electrodes, due to the need to remove the liquid dispersing media under very controlled conditions to get a homogeneous, uniform coating. Also, energy consumption for the evaporation process is high, significantly contributing to the carbon footprint of the overall cell manufacturing process. Li based batteries produced today are not designed specifically with recycling in mind therefore future battery designs and processes could improve sustainability by taking a circular economy mindset.

## 1.3.2 R&I NEEDS

- Increasing the yield while reducing the environmental impact (both in terms of emission and waste production) and energy efficiency / consumption are key targets for the European industry;
- Design for recycling at cell and cell component level;
- Innovation on process and manufacturing equipment should focus on improving current technology sustainability (material and energy efficiency, design for recycling);
- Adapting and developing environmentally friendly manufacturing processes using Generation 3 and 4 materials, including water based and solvent-free coating as well as design for recycling of cells and components;
- Implementation of circular economy, e.g. by reusing materials from different industries (e.g. steel industry Ni), by facilitating manufacturability, disassembly, recovery of components and recyclability;
- Facilitate not only the battery cell and battery module assembly but also the dismantling process to foster the second use and recycling process;
- New tools and comprehensive methodologies must be developed to perform environmental and Social Life Cycle Assessment (s-LCA).

## 1.4 WHAT IS NEEDED FOR EUROPE TO BE COMPETITIVE?

Batteries are a key technology that can contribute to the growth of countries by generating jobs, revenues and social wealth. There are also other added values that should go along R&I measures like the ones proposed in this Roadmap. For example, the commitment to responsible manufacturing. The European industry of the future has to ensure the implementation of due diligence obligations with regards to human and labour rights, as well as environmental protection throughout its supply chain. Production facilities have to be carefully located attending to local criteria such as production of renewable energies, availability of raw materials, refining and processing of active cathodes and anodes at that location, as well as local demand for integration into different applications. This will minimize the carbon footprint and the cost of the whole system. Many of these objectives will be subject to legal obligations under the new battery legislation that has been proposed by the European Commission and is currently being discussed with the European Parliament and the Council.

## 1.4.1 IMPACT

The efficient design of cells and its components will increase cell energy density while maintaining at least already existing safety levels.

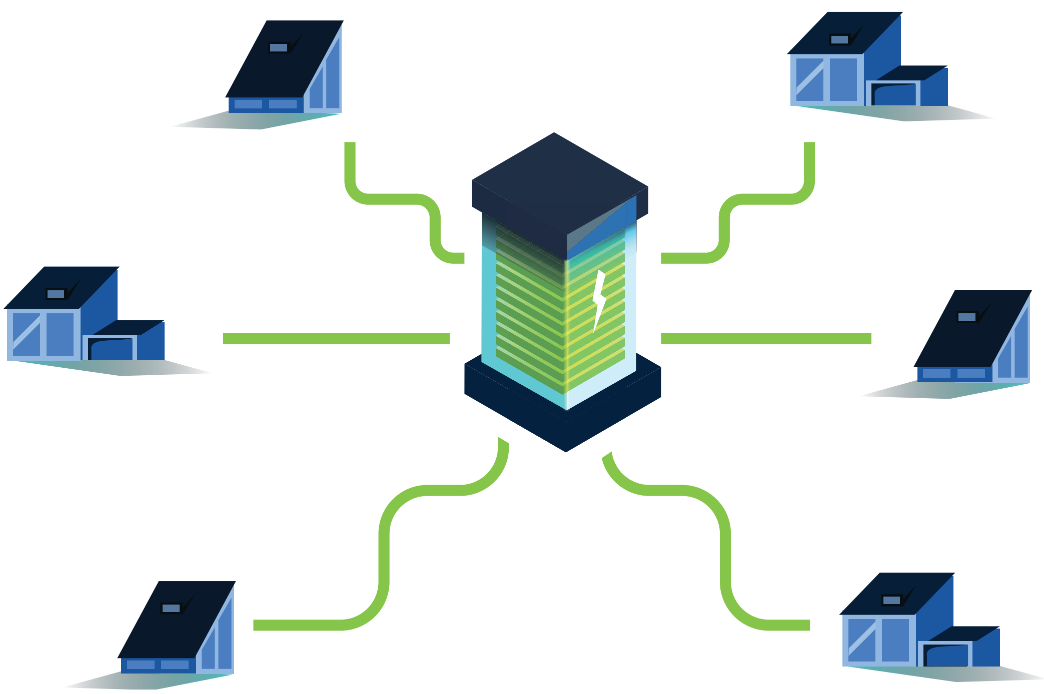
Green manufacturing techniques at cell component level, will decrease the environmental impact of the cell manufacturing process significantly. It will, on the one hand, decrease its carbon footprint to a level where $CO_2$ neutral manufacturing can be achieved. On the other hand, it will contribute to and make use of the circular economy by improving design for recycling and increase the quantity of materials sourced from recycling processes.

To achieve a design for recycling the first stage is to review all the processes associated to the entire life cycle and incorporate recyclability and social impact criteria into the design phase of a battery. It is absolutely necessary that battery manufacturers interact with recycling experts as early as possible to ensure a low effort recycling technology. This is the concept of “Design for recycling”. The potential recycling should be considered as early as possible on material, cell and battery level that is then added to other factors such as costs, safety and manufacturability. Design for recycling is a systematic approach allowing the manufacture of batteries with the lowest possible environmental footprint.

Implementing Generation 4 (all-solid-state battery) materials into the manufacturing process, with minimal adaptation needs, will bring solid state batteries and alternative chemistries closer to the market by decreasing the need for additional CAPEX for cell manufacturers. Solid-state electrolyte-based battery cells can increase the energy density and safety of cells by a large margin, but only when efficiently implemented at large cell level. The interface of all components is crucial for cycle life, stability, energy density and safety. Therefore, optimised and reproducible manufacturing will be the key to enable all-solid-state battery technology for wider market adoption.

## 1.4.2 RESOURCES REQUIRED

- Networks between pilot lines and production sites;
- Skilled personnel;
- In the 2020-2030 period it is recommended to deploy enough resources for developing, validating and demonstrating competitive EU manufacturing technology for current generation and next-generation batteries;
- Environmental policies could speed-up the R&I deployment. Higher efficiency, more sustainable manufacturing process and efficient manufacturing equipment should be promoted.



# 2. STRATEGIC TOPIC 2: DIGITALIZATION FOR CELL DESIGN, PROCESS INTEGRATION AT PRODUCTION LINE LEVEL AND PLANT OPERATIONS

## 2.1 CELL DESIGN DIGITALISATION

Digitalization of the battery cell design will result in both costs savings and performance improvement. Multiple digitalization tools will be used to tackle different challenges, including machine learning (ML) and artificial intelligence (AI) coupled to multi-physics models replacing the trial-and error approach to battery development. These tools will help to develop the understanding of battery cell behaviour and therefore provide the means to improve battery performances, lifetime, reliability and safety. These tools will also support assessing the environmental impact by monitoring key environmental KPIs, like CO2 footprint.

### 2.1.1 STATE OF THE ART

The production of battery electrodes and cells is a very complex process. As the quantitative influence of production parameters and their interdependencies are little understood yet, for the prediction of optimum production line set-up and operating parameters as well as the control of the interacting process steps, digital tools such as digital twins and industry 4.0 solutions have to be developed further. To enable this, new tools such as sensor implementation, facilitating the machine inter-connectivity and minimizing human monitoring, and digitalization, based on physical and/ or data-driven models (among others by using AI) are required. This means both precise and in-depth simulation methods/tools as well as short-cut models for real-time model-based control of the production lines.

Regarding simulation of cell performance, many approaches based on multi-physics (i.e. based on different physical and chemical principles) and multiscale (from atomistic to continuum scale) models can be identified in literature. There are certain works in the field of multiscale and multi-physics coupled models for cell simulation, where the parameters act as a link between the different scale models or different unit processes[4] [5]. Also, some approaches on reducing

[4] Kim et al., "Multi-Domain Modeling of Lithium-Ion Batteries Encompassing Multi-Physics in Varied Length Scales," J. Electrochem. Soc., 2011, Vol. 158, No. 8, pp. A955–A969
[5] Oke Schmidt et al 2020 J. Electrochem. Soc. 167 060501

computational cost can be found in literature, where the multi-physics models are either coupled to machine learning algorithms or structure models, so called as surrogate models[6]. However, there is not much information on the quantification of the reduction of experiments as a result of the model-based cell design.

The overall costs of the battery can be reduced significantly if digitalization approaches are successfully integrated in an automated production line as known from other industries (e.g. automotive). The use of sensors and actuators and their interaction with their environment is currently still limited to basic safety functions or automatic calibration of workpieces.

## 2.2 PROCESS INTEGRATION AT PRODUCTION AND PLANT LEVEL

Currently, considerations have to be taken towards a more integrated battery manufacturing eco-system, across country borders and neighbouring industries. This is a significant challenge in many European countries since the gross energy costs are high and still strongly associated with CO2 emissions.

A close integration with the local ecosystem is also important to secure a more efficient material flow within the battery value chain. A transformation into digitalized processes will be the key to unlock optimization potential across the battery value chain.

### 2.2.1 STATE OF THE ART

The excellence of battery plant operations strongly affects material costs and energy costs (ca. 90% of the OPEX). In this respect, beyond all measures which a battery manufacturing plant can conduct completely on its own, there is a very significant improvement potential in a tailored cooperation with other industries of the local ecosystem in order to jointly exploit sector coupling benefits and industrial cluster integration synergies. For the exploitation of these benefits, digitalization can be a key enabler.

This refers to implementation of digital hardware elements like smart meters and smart grids. This also enables the interaction of different industrial plants and an overarching optimization, using appropriate software which processes the data. Moreover, simulation of the entire plant including building services, especially dry room, will enable a knowledge-based plant operation with minimized energy consumption.

[6] Cui, T, Zheng, Z, & Wang, P. "Surrogate Model Assisted Lithium-Ion Battery Co-Design for Fast Charging and Cycle Life Performances." Proceedings of the ASME 2020 International Design Engineering Technical Conferences and Computers and Information in Engineering Conference. Volume 11B: 46th Design Automation Conference (DAC). Virtual, Online. August 17–19, 2020.

## 2.2.2 R&I NEEDS

- Coupling the multi-physics models with optimization algorithms to automatize the cell design and production process improvement;
- Coupling the multi-physics models to economical models, where the cost can be anticipated prior to manufacturing;
- Time-consuming calibration and parameterization of models;
- Translation of parameters from one modelling scale to another.

**Short term until 2025**

- Development of accurate, reliable and low computational cost models;
- Extraction of parameters from production lines for modelling and validation purposes;
- Digital methods based on reliable digital twins are required to predict the performance of giga-scale production lines based on pilot line results;
- Enabling traceability of production information along the process chain to make the production line transparent, among others with regard to a digital battery passport;
- Predictive and preventative maintenance based on data acquisition and model-based evaluation;
- Applicable model to exploit benefits from sector coupling, including creation of energy parks, as business model innovation.

**Medium-term until 2030**

- Deep model-based understanding of how the various process and machine parameters affect battery performance, costs and the environmental impact;
- "Standardized" model landscape should be defined (stabilising the protocols for validating the models, usage conditions, and so on);
- Development of advanced numerical approached for reducing the computation cost;
- Models to predict/segregate bad cells from good after production;
- Combining performance models with cost models;
- Optimization tool to improve battery plant material and energy flow ecosystems integration;
- Developing a blue print and a model for the simulation of optimized material and energy flow structures for battery plant integration;
- Simulation of different operation mode options and their impact on overall productivity and profitability using digital data;
- Assessing the potential impact of new battery technologies on sector coupling opportunities and industrial synergy exploitation.

**Long term 2030+**

- Digital twin on plant level including innovative concepts of air conditioning (humidity, particles), water handling, ...;
- Developing a digital twin of a battery manufacturing plant to assess best possible interaction with other elements in the battery value chain;
- Assessing the efficiency gain by transferring analogous process management elements to digital in time process optimization.

## 2.3 WHAT IS NEEDED FOR EUROPE TO BE COMPETITIVE?

For an efficient and world leading cell design comprehensive simulation tools, i.e. digital twins of cells are required which are based on active material morphologies and performance on particle level as well as microstructure an electrode and cell level. The goals of the digitalisation topic regarding cell design are mainly reducing cost by 20% and increasing the performance of the cells by 10% in terms of energy efficiency. In the long term, to reduce the time to market by reducing the development cycle by 30% which will help Europe to come first into the market with new cell technologies/ chemistries.

Battery cell production lines and plants are highly complex due to the vast number of parameters and only partly understood process-product cause-effect relations. Once successfully operating, production systems are rarely changed due to the risk of expensive production downtime, not knowing whether the production process has already achieved optimal product quality and maximum throughput. In order to: design, construct, operate and optimize economically and ecologically leading giga-scale production lines and plants with minimum scrap and maximum quality and output, a digital, knowledge-based approach is required. In the short to medium-term, digitalization is needed within the following three areas:

- Planning phase: virtual commissioning of the production line by dynamic 3D representations, including the product (electrodes, cells) to the process in the plant;
- Run phase: cell production by digitalization (manufacturing operations, guiding the field operators, Sensors and 5G technology to enable big data collection, quality monitoring and maintenance);
- Optimization phase: continuous improvement of the manufacturing operations, improvement of productivity with optimized planning and scheduling, reduction of scrap rate by improved quality monitoring.

Regarding plant operation, Europe must consider its specific industrial structures and develop a tailored model which exploits competitive benefits through the interaction of a battery plant with the local energy and materials ecosystem. Thus, Europe shall aim at: Site specific exploitation of sector coupling, through integration into existing industrial clusters reduction of supply chain and recycling costs and transformation of the analogous processes into digitalized processes.

Moreover, AI and other optimization tools shall be employed to optimize the system on plant level to gain minimum energy consumption, production scrap and environmental impact and in parallel maximum production capacity and cell performance. Finally, the multiscale digital twin shall be able to handle not only lithium-ion batteries, but also new generation like solid-state batteries.

## 2.3.1 IMPACT

The digitalization of the cell design methodology and the production line is highly essential to continue the improvement of battery design and production especially when facing the constantly occurring innovations (e.g. new cell design, chemistries, process technology). In the short to medium term (by 2030), digitalization will enable transparent battery production in which key parameters along the process chain are continuously recorded and analyzed so that machines can be controlled individually. Model-based results will help understand the cause-effect relations in battery production and provide decision support for operation. In the long term (by 2050), fully functional cyber-physical production systems must be implemented in battery production which provide a direct control and self-optimization of the entire process chain.

## 2.3.2 RESOURCES REQUIRED

- Initiatives to bring key players together for focussed research;
- Standardisation of models used for cell design to help in co-design activities;
- Better characterisation and inline sensor techniques – using analytical techniques to provide inputs for model development;
- Legal support or policy creation to solve IP issues to create more trust between various players;
- All digital technologies and tools have to be tested in pilot and industrial scale production lines.

# 3. PRIORITISATIONS & KEY RECOMMENDATIONS

Many challenges are yet to be overcome to establish a competitive battery production in Europe. As lithium-ion technology and its different generations will dominate the electrification landscape in the next years, special focus need to be put in this family of battery technologies. The high complexity of the battery cell and its production process requires an interdisciplinary approach in which European core competencies need to be bundled and extended to promote a successful battery design and production. Innovative cell components and design as well as manufacturing processes and machinery are fundamental to a continuously improving battery cell performance while simultaneously reducing costs and environmental impact. In addition, a digital, knowledge-based product development and production process must be promoted in order to avoid expensive trial-and-error operation.

Digitalization is a decisive enabler not only to uncover cause-effect relations within the battery cell and along the production line, but also to enable fully automated production lines and plant operation resulting in higher battery cell performances and production yields. Business model innovations are needed including sector coupling, e.g. creation of energy parks, digitalized models for a close cooperation with suppliers, customers and partners to jointly and continuously identify and implement improvements and synergies – especially in energy efficiency. Nevertheless, the entire life cycle must be included in the product design and the production process to foster a circular economy in which battery cells can be recycled at their end-of-life and the overall environmental impact is reduced to a minimum. Instead of stand-alone factory, battery factories must be integrated in local ecosystems in order to increase the overall efficiency of the factory and simultaneously decrease environmental impact to a minimum.

**Technology Development** - Innovation in battery cell components design, manufacturing equipment and processes

To be competitive with non-European countries, European-made batteries must not only achieve better performance (high energy density, fast charging capability), but also be safe and sustainable. Therefore, the choice of cell and component design to increase the energy density is a very decisive factor. Based on today lithium-ion battery technology Europe must develop deep knowledge to design optimum cells, especially their microstructure and interfaces, with future materials, such as solid electrolytes and lithium anodes or even lithium-free anodes. The acquisition of materials for cell components should take into account local, environmentally friendly supply chains in order to become independent of non-European countries, to raise quality standards in certain cases and to fulfil their due diligence obligations with regard to human and labour rights as well as environmental protection.

In order to be competitive Europe has to have a strong industry of machine and equipment supplies. This industry should have strong experience of the behaviour of their machines in the industrial environment and the most innovative yet robust and sustainable process and machinery solutions (as for example dry coating technology) with maximum yield and energy efficiency.

Moreover, the equipment and production lines should be flexible or transferable, respectively, with regard to upcoming cell generations. For the aspect of sustainability, a "design for recycling" needs to be applied at material, cell and battery level. Here, all processes associated with the entire life cycle are verified and criteria for recyclability and social impact are included in the design phase of a battery. For a quick implementation, recycling experts should be consulted. Following from this a circular economy should be established. In addition, environmentally friendly production of cell components (e.g. water-based or solvent-free coatings) is desirable.

**Digitalization** – Digital tools and twins for cell design, for process integration at production line level and for plant operations

In order to produce high-performance batteries with high efficiency, there is a need to develop models that can predict (on the basis of experimental data and rapid parameterisation methods) the compositions of the various battery components that will achieve the best energy densities and the lowest costs. Battery quality should be ensured through the implementation of a battery passport concept and the digital twinning of manufacturing and battery management through sensors, automation and AI process controls. This will ultimately lead to competitive battery performance and cost.

The planning, running and optimization of production lines shall be significantly improved regarding costs, productivity, product quality and environmental impact by digital tools and digital twins. In the medium and long term, multiscale digital twins of the entire giga-factories from material to plant level shall be used to predict plant, production line and battery cell performance, costs and environmental impact. Development, calibration, and validation of the digital twins require continuous acquisition of essential production parameters and product characteristics. Best-practices from other industries should be applied to speed up the digitalization process. Developing both mechanistic and data-based models is essential to identify, predict, and finally control the relevant process-product relations. For this purpose, cyber-physical production systems need to be implemented to enable a fully-automated material-efficient production process with high yields. Since the European industries have already vastly invested in automatisation in other sectors (e.g. automotive, food, pharmaceutical), synergies can be established to make use of the knowledge that has been generated. Production lines must be flexible against the background of ever-changing cell formats (cell formats, types) and new battery generations. In addition, artificial intelligence and machine learning need to be used in the future to accelerate the development of new processes and equipment. Transparent battery production and the establishment of a label for the total energy consumption of a battery system can help to make the production more sustainable and cheaper. Finally, digitalized models shall be applied for a close cooperation with suppliers, customers and partners to jointly and continuously identify and implement improvements and synergies – especially in energy efficiency.

# 4. CONCLUSIONS

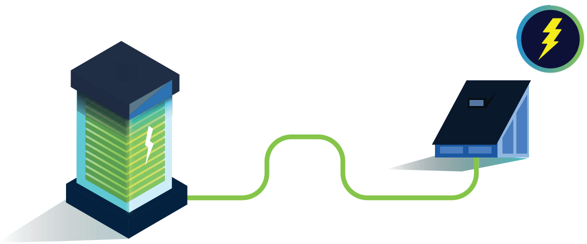
To be competitive with non-European countries, European-made batteries must not only achieve better performance -higher energy density, fast charging capability-, but also be safe and sustainable.

As the lithium ion and its different generations will dominate the electrification landscape in the next years, focusing the actions proposed in this Roadmap into them will maximize impact and resources utilisation. Battery technologies other than the lithium-ion family, may well be included in future revisions of this roadmap as the market evolution will call for them.

To achieve these targets, this Roadmap proposes a R&I strategy focusing into two strategic areas. The first line of action focuses on technology and equipment development, addressing new production technologies for current and new chemistries minimizing costs and environmental impact. At the same time, digitalization is addressed as a key horizontal approach addressing developments from the cell design, to equipment and production line digital twinning, up to plant site local ecosystem optimization.

As the perceived weakest link in the European battery value chain remains in cell design and manufacturing, no particular prioritization is done amongst the various technological approaches proposed in this Roadmap. On the contrary, we propose to take action along the full package of strategic technologies identified.

This approach, in close interaction with developments from strategic side actions such as Battery 2030+, will be at the foundations of the next generation of battery cell giga-factories in Europe.



# 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<br>Lion HC | Advanced<br>Lion HC | Solid State | | | Beyond Li-ion |
| Expected<br>Commercialisation | Commercialised | Commercialised | | 2020 | 2025 | >2025 | | | |
| Cathode | NMC/NCA<br>LFP<br>LMO | NMC111 | NMC424<br>NMC523 | NMC622<br>NMC811 | HE NMC<br>Li-rich NMC<br>HVS | NMC | NMC | HE<br>NMC | |
| Anode | Modifed<br>Gaphite<br>$Li_4Ti_5O_{12}$ | Modified<br>Graphite | Modified<br>Graphite | NMC910<br>Carbon<br>(Graphite)+Si | Silicon/Carbon<br>(C/Si) | Silicon/Carbon<br>(C/Si) | Li<br>metal | | Li<br>metal |
| Electrolyte | Organic<br>LiPF6salts | | | (5-10%) | Organic+<br>Additives | Solid electrolyte<br>-Polymer (+Additives)<br>-Inogranic<br>-Hybrid | | | |
| Separator | Porous Polymer<br>Membranes | | | | | | | | |

Source: Nationale Plattform Elektromobilität, Marcel Meeus, JRC.

# KPI Tables

| Manufacturing | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| Sustainable Manufacturing Processes | | | | | | | | | |
| Parameter | KPI | Operating conditions | Description | System/Pack level | Unit | Source, contribution | 2014-2015 | State of the art | 2030 Li-ion mass production scenario |
| | Energy consumption | | | | kWh/kWh | | | 100* | <25 |
| | CO2 footprint manufacturing (not materials) | | | | kgCO2eq/ kWh | | | 61-106* | 10 |
| | Capex | | Capital cost | | Mio€/GWh installed | Related to level of scale up | | 90 / 100 | 60 / 80 |
| | Opex | | Operational cost – assume excluding material | | €/kWh | | | 20 | 10 |
| | Scrap rate on cell level | | Yield, quality, utilisation of materials | | % yield | | | 85 | 95 |
| | Effectiveness of production | | Resources used (e.g. water and others) | | % | | | 70 | 90 |
| Cell design | | | | | | | | | |
| | Gravimetric energy density at cell level | | | | Wh/kg | | | | 300...450 |
| | volume energy density at cell level | | | | Wh/l | | | | 800...1000 |
| | Voltage level | | | | V | | | | |
| | Utilisation of theoretical capacity | | Capacity at cell level/ theoretical capacity active material, volume and mass | | | | | | xxx |
| | Total energy throuput | | | | kWh/kWh inst. | | | | |
| | Deep cycles for high capacity applications | | | | | | | | 2.000...80.000 |
| | deep cycles for high capacity applications | | | | | | | | |
| | C-Rate | | | | | | | | |
| | Cost at pack level | | | | €/kWh | | | | xxx |
| | Cost at cell level | | | | €/kWh | | | | 70...200 (Northvolt: 65) |

# References

See within text.