D2.3 Cell fabrication and module design specifications

JØRN DØVLING KASPERSEN
BYD

AMAIA SAENZ DE BURUAGA
BCARE

MARCEL WEIL / SEBASTIAN PINTO-BAUTISTA
KIT

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Checked by	Amaia Saenz de Buruaga (BCARE) Marcel Weil/Sebastián Pinto-Bautista (KIT)	2023-06-22 2023-06-22
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Publishable summary

Due to the global climate crises and an increasing demand of energy, the world is transitioning away from fossil fuels and towards a larger degree of electrification. In order be able to power more applications with electricity, more energy storage systems are being developed with the aim to cover the different applications. In this concern, batteries are a critical key technology for the transformation of energy and mobility sectors necessitated by the climate concerns. They can make a high contribution to the transition to a sustainable economy. However, considering the entire life of these batteries, their sustainability of both production and product along the entire value chain need also to be kept in mind, thus maximizing the contribution of these energy devices to a more sustainable and environmentally friendly economy.

Therefore, the MUSIC project aims to develop a sodium-ion capacitor which can provide more power than a conventional lithium-ion battery but at the same time has a higher energy density than a supercapacitor. However, for the applications using the developed technology to be more sustainable than today's available solutions, sustainability of the sodium-ion capacitor throughout its lifetime must be considered from the start of the project. Thus, the objective of this deliverable is to provide guidelines for sustainable sodium-ion capacitor cell manufacturing and eco-design module development. Additionally, some specifications of the sodium-ion capacitor cell to be developed in the MUSIC project will be provided.

In general, sustainability of any new energy storage device (or product in general) should be assessed using life cycle thinking, *i.e.* considering the environmental and human impact of the entire life cycle of the solution. For energy storage devices, this includes extraction/production of raw materials, manufacturing of the cells, incorporations of the cells into modules and battery systems, use phase, second use, and recycling at end of life.

It must be noted that not every "greener" choice will necessarily lead to overall better environmental performance. In fact, the technical performance of the device may result more decisive to determine its environmental profile. For example, the choice of a material with slightly larger environmental impacts per unit of mass than a "greener" alternative, but which leads to a significant increase in the energy density (with all other technical aspects remaining the same) will result in a decrease of the system size and number of cells to be produced, thereby reducing the specific environmental impacts per unit of storage capacity. The impact on technical performance should therefore always be considered (but not limited to) when attempting to improve the sustainability of the cells via changes in material selection. Early sustainability and technology assessments might then become fundamental for decision making within the development process. These might also reveal potential trade-offs between environmental and technical performance for specific applications, for instance, when the weight of the device is not a critical parameter or, on the contrary, when lightweight design is highly desired.

Despite of this, the developmental phase of new sodium-ion capacitor technology should also focus on minimizing the environmental and human impacts. Sustainability analyses should consider many different aspects, for example fossil depletion potential, global warming potential, terrestrial acidification potential, human toxicity potential, freshwater and marine eutrophication potential, metal depletion potential, and potential violations of human rights *etc*. The cell development phase should also consider using materials which require less energy usage in the cell manufacturing stage, easier repair, and/or easier recycling. Also the use of environmental guard rails, like e.g. decrease the use of critical/toxic materials, or not using per- and polyfluoroalkyl substances is quite important within the design phase.

In addition to the environment impacts of the cell design and raw materials, the production phase should also be optimized in terms of sustainability. This may for example include using renewable energy, optimizing the process to decrease the energy usage, and assure a high quality of the manufacturing process to increase the yield.

The same applied for the packing of the sodium-ion capacitor cells into modules. Additionally, the environmental impacts of the module and system should be decreased by making compact module design which are preferably adapted to specific applications, the materials should have low impacts, and all parts of the cells should be easy to repair and/or replace. However, a compact and application-specific design could be conflicting with increased recyclability and/or ease of repair, so it is necessary to include discussions of potential conflicting goals and identification of trade-offs.

In the use phase, a high charge and discharge efficiency will decrease the energy loss during cycling, resulting in lower impacts. If possible, conservative limits on charge/discharge rates and voltages could be set to extend the life of the cells. When the capacity of a module has decreased to a low cut-off value, the module should have a second use in another application with less strict performance requirements. Finally, the cells should be reused or recycled as much as possible, likely requiring development of new recycling methods for some materials.

To increase the overall sustainability of energy storage devices, sodium-ion capacitor manufacturers and module developers should engage in and support political work to increase the sustainability requirements by industry organizations and ruling authorities. For example, the sodium-ion capacitor manufactures should support the work being done on the Battery Passport by the Global Battery Alliance and EU's Battery Pass, which aims to increase the transparency of sustainability reports for energy storage systems and cells. In this way, every company is bound to satisfy certain sustainability requirements and provide further information, like *e.g.* carbon footprint.

In the MUSIC project, the goal is to improve sustainability of the metal-ion capacitor technology compared to state-of-the-art lithium-ion capacitors in two main ways: improving the energy and power density, thereby requiring less cells to be used for a given application, and replacing the high-impact materials graphite, copper, and lithium with the potentially more sustainable materials hard carbon (potentially from organic waste), aluminium, and sodium. Additionally, the pre-sodiation method is chosen to avoid extra energy-intensive steps in the manufacturing.

In addition to the preliminary sustainability considerations described in this document, the MUSIC project will include a full life cycle assessment and economic analysis to assess the full potential of the sodium-ion capacitor technology. The analyses will follow the natural sodium-ion capacitor cell and system development during MUSIC and include environmental and economic assessments of cell components at first, followed sequentially by first prototype, full device at industrial production, and system level including use case, second use, and recycling. The sodium-ion capacitor cell and module development can thereby be supported and directed by the parallel life cycle analysis performed, which is also preferably how research and development should be conducted by industry.

It is recommended that the general guidelines presented in this document are used by sodium-ion capacitor manufacturers and module developers as a basis for a sustainable development of the sodium-ion capacitor technology. In this way, sustainability aspects can be considered from the start of the technological development process, decreasing so the likelihood of spending large amounts of time and resources on technological pathways characterized with poor environmental performance. These guidelines should also be followed by the partners in the MUSIC project.

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Abbreviations

SYMBOL	**SHORTNAME**
BMS	Battery Management system
EMS	Energy Management System
EU	European Union
i-SMS	Innovative Supercapacitor Management System
LCA	Life Cycle Analysis
LIB	Lithium-ion Battery
LIC	Lithium-ion Capacitor
SIB	Sodium-ion Battery
NMP	N-Methyl-2-pyrrolidone
OEM	Original Equipment Manufacturer
PCB	Printed Circuit Board
SIC	Sodium-ion capacitor
SMS	Supercapacitor Management System
SMD	Surface Mount Devices
SoC	State of Charge
SoH	State of Health
SoP	State of Power
PFAS	Per- and polyfluoroalkyl substances

1 Introduction

Due to the global climate crises and an increasing demand of energy, the world is transitioning away from fossil fuels and towards a larger degree of electrification. In order be able to power more applications with electricity, more energy storage systems are being developed with the aim to cover the different applications. In this concern, batteries are a critical key technology for the transformation of energy and mobility sectors necessitated by the climate concerns. They can make a high contribution to the transition to a sustainable economy. However, considering the entire life of these batteries, their sustainability of both production and product along the entire value chain needs also to be kept on mind, thus maximizing the contribution of these energy devices to a more sustainable and environmentally friendly economy.

The MUSIC project aims to develop a sodium-ion capacitor (SIC) which can provide more power than a conventional lithium-ion battery (LIB) but at the same time has a higher energy density than a supercapacitor. However, for the applications using the developed technology to be more sustainable than today’s solution, sustainability of the SIC throughout its lifetime, must be considered from the start of the project.

The objective of this deliverable is to provide guidelines for sustainable SIC cell manufacturing and eco-design as described in task 2.3 of the MUSIC proposal, as well as to provide some SIC cell and module specifications as suggested in the title of this deliverable. The general guidelines are provided first, followed by cell and module specifications. The discussion section elaborates on the cell design choices and materials which have been considered as a starting point for upscaling to a large format cell.

This deliverable aims to ensure that sustainability aspects of the SIC are considered from the beginning of the technology development process. This will decrease the risk of focusing the development on a technological direction with high environmental impacts.

Sustainability is an intricate topic which includes considerations and relative weighting of many different impact categories, and good, data-driven decisions require complex and prospective life cycle analysis (LCA) studies to be performed. Therefore, the MUSIC project incorporates LCA studies of different aspects of the SIC technology, including environmental and economic assessment of the cell constituents, at prototype cell level, at industrial production level, and at system level considering manufacturing, use case, second use, and recycling. These LCA analyses will provide valuable information of the sustainability profile of the SIC technology and may help to identify economic and environmental hotspots and will support its development in the most sustainable direction from a full life cycle point of view. These guidelines suggest a similar approach when research and development is performed in the industry.

2 Methods and Results

This section provides information in terms of general guidelines that sodium-ion capacitor cell manufacturers as well as module developers should take into consideration to optimize the environmental performance of the technology in its various life cycle stages, from the design and production to the end-of life. Only one publicly available study on metal-ion capacitors has been identified[1] (an LCA study on lithium-ion capacitor (LIC) containing activated carbon and lithium titanium oxide), so the general guidelines are inspired by the work from the battery sector. The guidelines align well with the "safe and sustainable by design chemicals and materials" framework recently presented by the European Commission's Joint Research Centre[2].

In addition to general guidelines, this section will also include specifications of the plans for the cell and module fabrication in MUSIC project.

2.1 Sustainability considerations

In this section, general guidelines that sodium-ion capacitor cell manufacturers and module developers should follow are addressed.

2.1.1 Cell design and material selection

Production or extraction of any material, particularly for energy storage devices, will have an impact the environment. Therefore, one of the main points of focus during the design, development and planning of energy storage devices should be the performance and lifetime of the device in relation to its application. For example, if the cycle life of an energy storage device can be doubled, the environmental impact (and cost) per total amount of energy storage during the lifetime of the device will be approximately halved[3], at least if the lifetime of the application is long enough to exploit the prolonged lifetime of the device. The same is true for a doubling of energy density of the device, which will result in half the number of cells needed to be manufactured. This effect should therefore be kept in mind for any attempt to improve the sustainability of an energy storage device; even if a change improves the sustainability slightly during production, *e.g.* using a material which is associated with slightly lower emissions of greenhouse gases, but significantly decreases the energy density or cycle life, the change may actually decrease the overall sustainability of the device.

Even though performance should always be kept in mind, material selection and cell design and development should preferably try to minimize the environmental impact of its eventual production, and try to select non-toxic, or at least less-toxic, materials such as using per- and polyfluoroalkyl substances (PFAS). This is not a straightforward process given the complex interconnections and the interaction between technology developers (battery designers) and system analytic experts. In addition, potential divergent results of different sustainability categories need to be addressed and recommendations deduced. Additionally, the relative weight of different sustainability aspects on the final assessment should be considered[4,5]. A preliminary sustainability screening of raw materials or components could be beneficial in this respect[6].

One aspect to consider is the environmental impact of each constituent in the cell. For instance, if two alternative materials with different environmental impacts result in the same performance of the energy storage device and do not require major changes in the cell production process, the material with the lowest environmental impact should preferably be chosen. Environmental impacts may for example include aspects such as fossil depletion potential, global warming potential, terrestrial acidification potential, human toxicity potential, freshwater and marine eutrophication potential, and/or metal depletion potential. Avoiding the use of materials from the EU's list of critical raw materials[7] may also be advantageous, though this list is more directed towards political decisions for investments in the raw material production within EU than as guidance for technology development.

A second important aspect to consider within the supply chain of any material relates to social impacts, which may potentially include human right violations. For example, mining of cobalt used in some type of LIBs (but not in the SIC developed in MUSIC) is known to be associated in some regions with child labour and poor working conditions[8]. Therefore, it is important to perform a thorough due diligence of the raw material suppliers, particularly from conflict-affected and high-risk areas[9], to ensure that the production or extraction of the used materials is not connected to violation of human rights or rise ethical questions.

In addition to technical performance and potential environmental and social impacts of the production/extraction of raw materials, the potential effects of selected materials on the production processes should also be considered as this could lead, among other things, to changes of energy demand during manufacturing. For example, since drying accounts for a large amount of the energy used in the production[10], dry manufacturing methods may be utilized or developed to decrease the total energy demand. Alternatively, materials which allow water-based slurries to be used instead of hazardous materials such as N-Methyl-2-pyrrolidone (NMP) may be selected, since the latter requires an energy-intensive system for NMP recovery.

Finally, if possible, the cell design should consider potential refurbishing of the cell to extend the use phase. One example, though likely difficult to achieve in large-scale production, may be to develop an appliance in the cell which allows for easy refilling of electrolyte to compensate losses due to side reactions during use.

2.1.2 Cell production

The production process of energy storage cells is generally associated with high energy consumption, particularly the drying process and energy use connected with dry rooms[10]. As for LIBs and sodium-ion batteries (SIBs), SICs will utilize a large potential window, so drying and use of dry rooms are important to avoid side reactions from residual moisture. Sustainability considerations and optimizations regarding the production process may therefore potentially have a large impact on the environmental profile of the cell.

First of all, the electricity provider and share of renewable energy in the electricity mix should be considered when deciding on where to install new large-scale production facilities, typically referred to as gigafactories. Locations with a high share of renewable energy in the mix should then be preferred. In addition, steps may be taken to optimize the production process, for example by implementing a large degree of digitalization tools, *e.g.* digital twins of the process and produced devices. Digitalization may allow the identification of relevant data reflecting correlations between performance variations and the production process. Furthermore, the production process may be planned and controlled in real time to decrease peak energy requirements of the process, which may both decrease electricity costs for the manufacturer and avoid the need for costly investments in the local electricity grid. An integrated system may also make it possible to harvest and re-use energy (energy recovery) from some of the production processes, for example heating/cooling exchange, recuperation of energy when slowing down movable parts of the line or reusing the energy from discharging cells during processes such as cell testing or capacity measurements. Since the large-scale factories are typically connected with large production volumes and a large amount of energy usage, even relatively small optimization may result in a significant energy saving.

In addition to the energy requirement of the production process, quality control at each step is also important to ensure adequate performance of the cells and to decrease the scrap rate. A larger total yield of cells means a lower specific environmental impact of each accepted cell, as the impact of the discarded cells would be added up to the average impact of the accepted ones. Since there is also a continuous development in production equipment, manufacturers of energy storage devices should follow this development closely while remaining flexible and innovative to quickly adopt technological improvements which may consequently increase the sustainable character of the production process.

2.1.3 Module design

Life cycle thinking should also be taken into consideration during design and development of the modules. A strategy in this sense is the design of compact modules that minimize material use (but consider at the same time also design for recycling and easy to repair issues). This way, the volumetric and/or gravimetric energy density of the module, and thereby of the energy storage system, can be maximized. This may consequently decrease the total demand of materials for a specific application and in some cases, *e.g.* electromobility, will also possibly lower the energy required to power that application due to a lighter and/or more compact design. For the same reasons, it may be beneficial in many situations from an environmental point of view to design the module specifically to the desired application, with an *ad-hoc* solution. Additionally, the module should be designed so that it is relatively easy to repair and replace, not only the cells, but also other components such as electronics, casing, and wiring. Moreover, the module may preferably be designed with parts which can be reused after the end of life, as well as incorporate secondary materials in its conception. Preferentially, the environmental impact of the materials used for the module should also be assessed, and the most sustainable options should be chosen.

2.1.4 Use phase

Sustainability of the use phase is more challenging to be addressed by the cell or module manufactures and must be addressed in a prospective manner for a potential application field. Apart from decreasing the self-discharge and increasing the efficiency during charge and discharge cycles to save energy, a focus may be to the extension of the cycle life of the cells. This may be achieved by setting conservative parameters in the Battery Management System (BMS) and/or Energy Management System (EMS), if the application allows it, since higher charge/discharge rates and higher/lower State of Charge (SoC) may accelerate the degradation of the storage device, ultimately shortening its cycle life. The BMS is responsible for safe operation, performance, and battery life under different working parameters such as operating temperature and current. Thus, a proper design of the BMS could extend the cycle life of a module reducing so its specific environmental impacts. The design of a very efficient BMS for supercapacitors could save also the usage of critical raw materials for electronic. Advanced algorithms or machine learning may be exploited by the EMS to learn from previous use cases when full performance is required and when more conservative parameters can be used to extend the cycle life. In addition, real-time estimations of battery SoC, State of Health (SoH), and State of Power (SoP), despite challenging, are very important for the application. This not only allows for battery fault diagnosis and prevention of hazardous accidents, but it also provides information on the battery performance that can support energy management optimizing consumption and lifetime. Moreover, with a real-time SoH estimation, battery maintenance and replacements can also be scheduled.

2.1.5 End of life

After the energy storage system has reached its end of life as initially defined, it should be properly disposed of. Ideally, the energy storage module should be suitable for second use in applications with lower requirements of energy density and/or specific energy, for example for grid stabilization in places where large space is available. Second use applications are already considered by the European Commission in the proposal for the EU regulation concerning batteries and waste batteries[11], where it has been stated that, at the end of the first life, batteries are not considered as waste but as new products.

After end of life of second use, the cells should be recycled complying at least with the corresponding rates set in the proposal for the new EU regulation concerning batteries and waste batteries[11]. Since cell manufacturers carry the most knowledge about their products, they could potentially take the responsibility for the recycling of their cells. Some cell/module components may be directly recycled, while others may require pretreatments to be broken down into smaller constituents or to eliminate toxic materials (*e.g.* PFAS). For some energy storage materials, the individual material constituents may represent a relatively low value, whereby recycling processes for these materials have not yet been developed. It may therefore be necessary to develop novel recycling processes for sufficient and cost-effective recycling.

2.1.6 Political engagement

To strengthen sustainability within the field of energy storage devices in general, and SIC in particular, SIC manufactures should engage in political work to increase performance standards and ensure possibilities for recycling. In this respect, SIC manufacture could be more active in similar EU activities like BEPA , Batteries Europe, or Batteries 2030+. If all manufacturers of energy storage devices are required to follow a basic set of sustainability regulations, it could be ensured that competition between different manufacturers from different geographical regions will not lead to compromising environmental performance to decrease cost and increase sale and/or revenue. For example, the SIC manufactures should support the work being done on the Battery Passport[12] by the Global Battery Alliance and EU's Battery Pass[13], which aims to increase the transparency of sustainability reports for energy storage systems and cells. In particular, The Global Battery Alliance has published a rulebook about global harmonized guidelines for adequate and transparent reporting of carbon footprint[14] (as one of many important environmental impacts), as well as a method for calculating human right indexes[15].

This type of initiatives will make easier for customers to choose between energy storage systems not comprising materials associated to *e.g.* child labour or poor environmental performance. In addition, SIC manufactures and module developers should support the development of standards and labelling for production of SICs and other energy storage cells, whereby it may become easier for OEM's to include cells from different manufactures, and for recycling companies to recycle different cells.

2.2 MUSIC cell fabrication specifications

In this section, cell specifications that sodium-ion capacitor cell manufacturers should follow are addressed.

2.2.1 Cell design, physical parameters

The sodium-ion capacitor cells to be produced in large format within the MUSIC project are planned to be fabricated in a pouch cell format with the overall dimensions as indicated in Figure 1. The cell thickness will depend on the thickness of the individual electrodes to be developed within the project, but it is expected to be around 6.9 mm to match a pouch size currently used in BYD's production facility. The pouch will comprise aluminium, and both tabs will be of aluminium with a thickness of 0.5 mm.

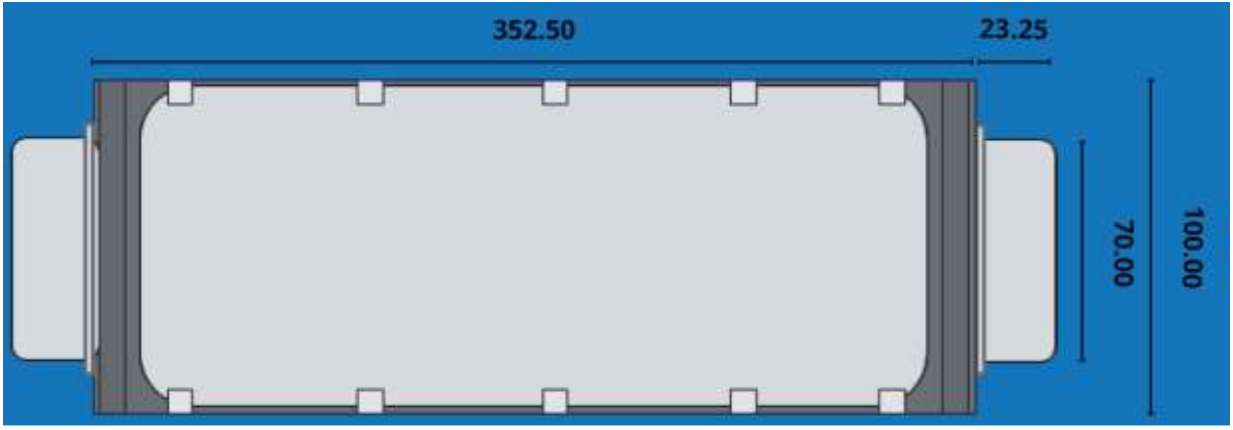


Figure 1: Cell design with dimensions in mm.

2.2.2 Cell design, materials

The detailed recipe of the constituents of the cell to be produced in large format will be developed during the project, particularly in "WP5: Electrode development and prototype fabrication". However, to decrease the risk of meeting unforeseen problems associated with novel materials during upscaling of the cell format, the large cells to be produced will be based on known materials. The cathode active materials will include super activated carbon, the pre-sodiation sacrificial salt will be $Na_2C_4O_4$, and the anode active material will be hard carbon. Sodium carboxymethylcellulose will likely be used as a binder, and carbon black is expected to be used as conductive additive. The electrolyte will include $NaPF_6$ in carbonate mixtures, though the possibility of using fluorine-free salts will be investigated during the project. The separator will be cellulose, and both electrodes will be aluminium foil, possibly surface-treated and/or carbon-coated.

2.2.3 Fabrication specifications

The SIC cells will be produced on a pilot production facility. Planetary mixers of 30 L or 45 L will be used to produce the slurries for the positive and negative electrodes. The slurry for the positive electrode will include the sacrificial salt for pre-sodiation. The slurries will be coated on both sides of aluminium foil rolls of 100 m in length using a transfer coater followed by drying in an oven. The electrode rolls will then be die-cut into individual electrodes of the desired size, and stacking of the electrodes will be performed by an automatic stacking machine. The cell stack will then be combined with the tabs and the pouch and welded together. The pouch will include a gas pocket to capture gas released during the step of formation/pre-sodiation.

2.3 MUSIC module design specifications

In this section, module specifications that sodium-ion capacitor module developers should follow are addressed.

2.3.1 Module design, materials

For the module design, the detailed information will be developed during the project, particularly in WP7. The different materials needed for the module design will be chosen in a way their environmental impact is considered. Four different main components are needed for the module development. In terms, the design specifications have already been explained in section "2.1 Sustainability considerations

In this section, general guidelines that sodium-ion capacitor cell manufacturers and module developers should follow are addressed.

2.3.2 Cell design and material selection

Production or extraction of any material, particularly for energy storage devices, will have an impact the environment. Therefore, one of the main points of focus during the design, development and planning of energy storage devices should be the performance and lifetime of the device in relation to its application. For example, if the cycle life of an energy storage device can be doubled, the environmental impact (and cost) per total amount of energy storage during the lifetime of the device will be approximately halved[3], at least if the lifetime of the application is long enough to exploit the prolonged lifetime of the device. The same is true for a doubling of energy density of the device, which will result in half the number of cells needed to be manufactured. This effect should therefore be kept in mind for any attempt to improve the sustainability of an energy storage device; even if a change improves the sustainability slightly during production, *e.g.* using a material which is associated with slightly lower emissions of greenhouse gases, but significantly decreases the energy density or cycle life, the change may actually decrease the overall sustainability of the device.

Even though performance should always be kept in mind, material selection and cell design and development should preferably try to minimize the environmental impact of its eventual production, and try to select non-toxic, or at least less-toxic, materials such as using per- and polyfluoroalkyl substances (PFAS). This is not a straightforward process given the complex interconnections and the interaction between technology developers (battery designers) and system analytic experts. In addition, potential divergent results of different sustainability categories need to be addressed and recommendations deduced. Additionally, the relative weight of different sustainability aspects on the final assessment should be considered[4,5]. A preliminary sustainability screening of raw materials or components could be beneficial in this respect[6].

One aspect to consider is the environmental impact of each constituent in the cell. For instance, if two alternative materials with different environmental impacts result in the same performance of the energy storage device and do not require major changes in the cell production process, the material with the lowest environmental impact should preferably be chosen. Environmental impacts may for example include aspects such as fossil depletion potential, global warming potential, terrestrial acidification potential, human toxicity potential, freshwater and marine eutrophication potential, and/or metal depletion potential. Avoiding the use of materials from the EU's list of critical raw materials[7] may also be advantageous, though this list is more directed towards political decisions for investments in the raw material production within EU than as guidance for technology development.

A second important aspect to consider within the supply chain of any material relates to social impacts, which may potentially include human right violations. For example, mining of cobalt used in some type of LIBs (but not in the SIC developed in MUSIC) is known to be associated in some regions with child labour and poor working conditions[8]. Therefore, it is important to perform a thorough due diligence of the raw material suppliers, particularly from conflict-affected and high-risk areas[9], to ensure that the production or extraction of the used materials is not connected to violation of human rights or rise ethical questions.

In addition to technical performance and potential environmental and social impacts of the production/extraction of raw materials, the potential effects of selected materials on the production processes should also be considered as this could lead, among other things, to changes of energy demand during manufacturing. For example, since drying accounts for a large amount of the energy used in the production[10], dry manufacturing methods may be utilized or developed to decrease the total energy demand. Alternatively, materials which allow water-based slurries to be used instead of hazardous materials such as N-Methyl-2-pyrrolidone (NMP) may be selected, since the latter requires an energy-intensive system for NMP recovery.

Finally, if possible, the cell design should consider potential refurbishing of the cell to extend the use phase. One example, though likely difficult to achieve in large-scale production, may be to develop an appliance in the cell which allows for easy refilling of electrolyte to compensate losses due to side reactions during use.

2.3.3 Cell production

The production process of energy storage cells is generally associated with high energy consumption, particularly the drying process and energy use connected with dry rooms[10]. As for LIBs and sodium-ion batteries (SIBs), SICs will utilize a large potential window, so drying and use of dry rooms are important to avoid side reactions from residual moisture. Sustainability considerations and optimizations regarding the production process may therefore potentially have a large impact on the environmental profile of the cell.

First of all, the electricity provider and share of renewable energy in the electricity mix should be considered when deciding on where to install new large-scale production facilities, typically referred to as gigafactories. Locations with a high share of renewable energy in the mix should then be preferred. In addition, steps may be taken to optimize the production process, for example by implementing a large degree of digitalization tools, *e.g.* digital twins of the process and produced devices. Digitalization may allow the identification of relevant data reflecting correlations between performance variations and the production process. Furthermore, the production process may be planned and controlled in real time to decrease peak energy requirements of the process, which may both decrease electricity costs for the manufacturer and avoid the need for costly investments in the local electricity grid. An integrated system may also make it possible to harvest and re-use energy (energy recovery) from some of the production processes, for example heating/cooling exchange, recuperation of energy when slowing down movable parts of the line or reusing the energy from discharging cells during processes such as cell testing or capacity measurements. Since the large-scale factories are typically connected with large production volumes and a large amount of energy usage, even relatively small optimization may result in a significant energy saving.

In addition to the energy requirement of the production process, quality control at each step is also important to ensure adequate performance of the cells and to decrease the scrap rate. A larger total yield of cells means a lower specific environmental impact of each accepted cell, as the impact of the discarded cells would be added up to the average impact of the accepted ones. Since there is also a continuous development in production equipment, manufacturers of energy storage devices should follow this development closely while remaining flexible and innovative to quickly adopt technological improvements which may consequently increase the sustainable character of the production process.

2.3.4 Module design

Life cycle thinking should also be taken into consideration during design and development of the modules. A strategy in this sense is the design of compact modules that minimize material use (but consider at the same time also design for recycling and easy to repair issues). This way, the volumetric and/or gravimetric energy density of the module, and thereby of the energy storage system, can be maximized. This may consequently decrease the total demand of materials for a specific application and in some cases, *e.g.* electromobility, will also possibly lower the energy required to power that application due to a lighter and/or more compact design. For the same reasons, it may be beneficial in many situations from an environmental point of view to design the module specifically to the desired application, with an *ad-hoc* solution. Additionally, the module should be designed so that it is relatively easy to repair and replace, not only the cells, but also other components such as electronics, casing, and wiring. Moreover, the module may preferably be designed with parts which can be reused after the end of life, as well as incorporate secondary materials in its conception. Preferentially, the environmental impact of the materials used for the module should also be assessed, and the most sustainable options should be chosen.

2.3.5 Use phase

Sustainability of the use phase is more challenging to be addressed by the cell or module manufactures and must be addressed in a prospective manner for a potential application field. Apart from decreasing the self-discharge and increasing the efficiency during charge and discharge cycles to save energy, a focus may be to the extension of the cycle life of the cells. This may be achieved by setting conservative parameters in the Battery Management System (BMS) and/or Energy Management System (EMS), if the application allows it, since higher charge/discharge rates and higher/lower State of Charge (SoC) may accelerate the degradation of the storage device, ultimately shortening its cycle life. The BMS is responsible for safe operation, performance, and battery life under different working parameters such as operating temperature and current. Thus, a proper design of the BMS could extend the cycle life of a module reducing so its specific environmental impacts. The design of a very efficient BMS for supercapacitors could save also the usage of critical raw materials for electronic. Advanced algorithms or machine learning may be exploited by the EMS to learn from previous use cases when full performance is required and when more conservative parameters can be used to extend the cycle life. In addition, real-time estimations of battery SoC, State of Health (SoH), and State of Power (SoP), despite challenging, are very important for the application. This not only allows for battery fault diagnosis and prevention of hazardous accidents, but it also provides information on the battery performance that can support energy management optimizing consumption and lifetime. Moreover, with a real-time SoH estimation, battery maintenance and replacements can also be scheduled.

2.3.6 End of life

After the energy storage system has reached its end of life as initially defined, it should be properly disposed of. Ideally, the energy storage module should be suitable for second use in applications with lower requirements of energy density and/or specific energy, for example for grid stabilization in places where large space is available. Second use applications are already considered by the European Commission in the proposal for the EU regulation concerning batteries and waste batteries[11], where it has been stated that, at the end of the first life, batteries are not considered as waste but as new products.

After end of life of second use, the cells should be recycled complying at least with the corresponding rates set in the proposal for the new EU regulation concerning batteries and waste batteries[11]. Since cell manufacturers carry the most knowledge about their products, they could potentially take the responsibility for the recycling of their cells. Some cell/module components may be directly recycled, while others may require pretreatments to be broken down into smaller constituents or to eliminate toxic materials (*e.g.* PFAS). For some energy storage materials, the individual material constituents may represent a relatively low value, whereby recycling processes for these materials have not yet been developed. It may therefore be necessary to develop novel recycling processes for sufficient and cost-effective recycling.

2.3.7 Political engagement

To strengthen sustainability within the field of energy storage devices in general, and SIC in particular, SIC manufactures should engage in political work to increase performance standards and ensure possibilities for recycling. In this respect, SIC manufacture could be more active in similar EU activities like BEPA , Batteries Europe, or Batteries 2030+. If all manufacturers of energy storage devices are required to follow a basic set of sustainability regulations, it could be ensured that competition between different manufacturers from different geographical regions will not lead to compromising environmental performance to decrease cost and increase sale and/or revenue. For example, the SIC manufactures should support the work being done on the Battery Passport[12] by the Global Battery Alliance and EU's Battery Pass[13], which aims to increase the transparency of sustainability reports for energy storage systems and cells. In particular, The Global Battery Alliance has published a rulebook about global harmonized guidelines for adequate and transparent reporting of carbon footprint[14] (as one of many important environmental impacts), as well as a method for calculating human right indexes[15].

This type of initiatives will make easier for customers to choose between energy storage systems not comprising materials associated to *e.g.* child labour or poor environmental performance. In addition, SIC manufactures and module developers should support the development of standards and labelling for production of SICs and other energy storage cells, whereby it may become easier for OEM's to include cells from different manufactures, and for recycling companies to recycle different cells.

MUSIC cell fabrication specifications". In the case of all the electronics needed for the SMS development, due to a lack of electronic factories in Europe, components are foreseen to be bought from the Asian market, which increases the environmental impact. In terms of wiring materials, km-zero wirings are expected to be used, thus reducing the emissions associated to transportations. Finally, regarding packaging of the cells, this will depend on the final product fabricated during the project, as well as the technical aspects of the module in terms of voltages (12V module expected) and capacity. However, second use plastic pack could be considered, as well as the use of additive manufacturing. If more materials are needed in order to have a mechanically robust and well-performing module, their environmental impact will also be assessed.

2.3.8 Fabrication specifications

For the module fabrication, different steps should be considered. As a first design of the module, which will depend on the final cell information as well as the module requirements, the following reference can be used:

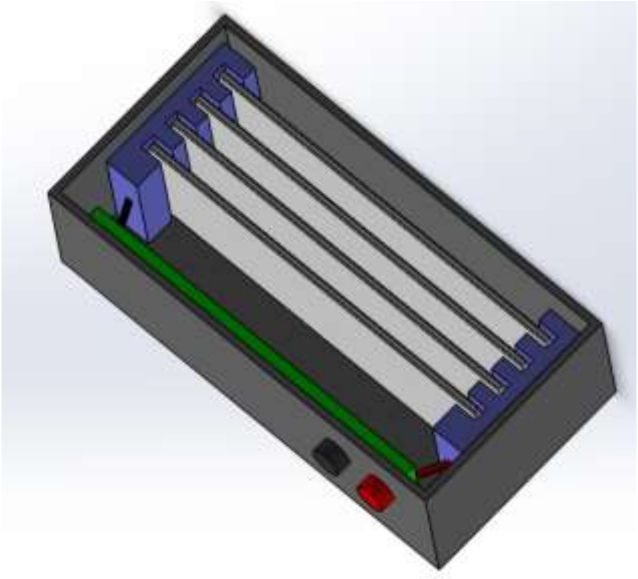


Figure 2: Prototype module design

In terms of the packaging (*in black*), this will depend on the final cell dimensions. Different options could be chosen, considering the additive manufacturing technique as well as second use plastic packs (if available in the market with the required dimensions) as viable options due to the prototype level of fabrication. In terms of cells (*in grey*), they will be developed by BYD following the above-mentioned fabrication specifications. For the fabrication of SMS (*in green*), once the different electronic components for the systems are chosen, as well as the electrical circuit, the Printed Circuit Board (PCB) will be fabricated. In this sense, two different components have to be considered: on the one hand, the Surface Mount Devices (SMD) which directly mount on the surface of the PCB and, on the other hand, the through-hole components, which have pins that are inserted into holes of the PCB and have to be welded to the board. The cells and the corresponding SMS need to be connected through cabling (*in red*) with positive and negative terminals. Finally, the enclosure cover will be provided with the corresponding positive and negative terminals.

2.3.9 Safety output

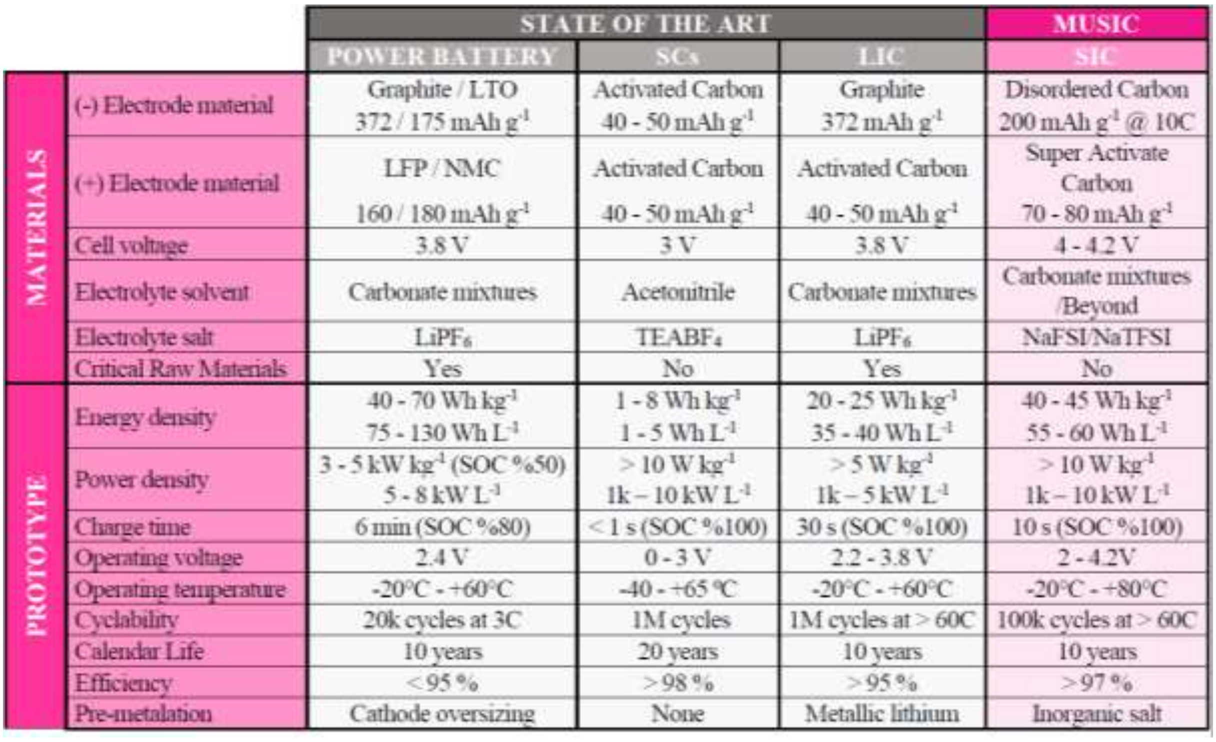
In terms of safety of the SIC module, the Innovative Supercapacitor Management System (i-SMS) will ensure safety of the system. Thus, the 12V module with the incorporation of sensors in the SMS will provide an intelligent system. Individual cell sensing will allow the registration of the voltage, temperature and impedance spectra of each cell in order to generate the corresponding SoC, SoH and SoP estimation models. These models will be based on cell experimental information extracted from the SIC cell performance under different operating conditions (currents, temperatures…). These performance tendences will be analysed in order to define the algorithms. The novel i-SMS will support safety operation of the module by limiting high values out of the protection limits in terms of temperatures, voltages, and currents by means of the integration of electrical protection circuit integrated in its hardware. In addition, a preliminary analysis of the thermal behaviour of the cell and module will be performed to evaluate the possible need of a thermal management system in future prototypes.

3 Discussion and Conclusions

The MUSIC project follows two parallel development paths: one path for upscaling currently available material to large format cells and module, and another path to develop novel materials. This document does not go into detailed LCA of the cell and module but provides just a few comments concerning the sustainability considerations of the selected available materials and possible novel developments.

As mentioned above, one of the main drivers for many sustainability aspects of an energy storage device is its technical performance. The perfect energy storage device should have both high gravimetric and volumetric specific energy, high cycle and calendar life, and high efficiency. In this way fewer cells would have to be used and manufactured for a given application (and therefore less resources used on system level), the cells would not need to be replaced, and the energy losses during the use phase would be low. However, battery materials generally have a higher specific energy but a lower power capability, cycle life, and efficiency. Supercapacitor materials have the opposite attributes, and metal-ion capacitors try to bridge the cap by providing intermediate performance between the two extremes. The most sustainable option will often be the one which matches the requirements of the specific application, with maximum utilization of the resources and energy used during manufacturing of the system. Development and commercialization of metal-ion capacitors may therefore improve sustainability of different applications by making a more suitable energy storage device available.

In the music project, the goal is to improve sustainability of the metal-ion capacitor technology compared to state-of-the-art lithium-ion capacitors in two ways.



		STATE OF THE ART			MUSIC
		POWER BATTERY	SCs	LIC	SIC
MATERIALS	(-) Electrode material	Graphite / LTO 372 / 175 mAh g^{-1}	Activated Carbon 40 - 50 mAh g^{-1}	Graphite 372 mAh g^{-1}	Disordered Carbon 200 mAh g^{-1} @ 10C
	(+) Electrode material	LFP / NMC 160 / 180 mAh g^{-1}	Activated Carbon 40 - 50 mAh g^{-1}	Activated Carbon 40 - 50 mAh g^{-1}	Super Activate Carbon 70 - 80 mAh g^{-1}
	Cell voltage	3.8 V	3 V	3.8 V	4 - 4.2 V
	Electrolyte solvent	Carbonate mixtures	Acetonitrile	Carbonate mixtures	Carbonate mixtures /Beyond
	Electrolyte salt	LiPF$_6$	TEABF$_4$	LiPF$_6$	NaFSI/NaTFSI
	Critical Raw Materials	Yes	No	Yes	No
PROTOTYPE	Energy density	40 - 70 Wh kg^{-1} 75 - 130 Wh L^{-1}	1 - 8 Wh kg^{-1} 1 - 5 Wh L^{-1}	20 - 25 Wh kg^{-1} 35 - 40 Wh L^{-1}	40 - 45 Wh kg^{-1} 55 - 60 Wh L^{-1}
	Power density	3 - 5 kW kg^{-1} (SOC %50) 5 - 8 kW L^{-1}	> 10 W kg^{-1} 1k – 10 kW L^{-1}	> 5 W kg^{-1} 1k – 5 kW L^{-1}	> 10 W kg^{-1} 1k – 10 kW L^{-1}
	Charge time	6 min (SOC %80)	< 1 s (SOC %100)	30 s (SOC %100)	10 s (SOC %100)
	Operating voltage	2.4 V	0 - 3 V	2.2 - 3.8 V	2 - 4.2V
	Operating temperature	-20°C - +60°C	-40 - +65 °C	-20°C - +60°C	-20°C - +80°C
	Cyclability	20k cycles at 3C	1M cycles	1M cycles at > 60C	100k cycles at > 60C
	Calendar Life	10 years	20 years	10 years	10 years
	Efficiency	< 95 %	> 98 %	> 95 %	> 97 %
	Pre-metalation	Cathode oversizing	None	Metallic lithium	Inorganic salt

Figure 3: Key Performance Indicators of current supercapacitor technologies and those aimed for MUSIC project

Firstly, the energy density will be improved from 20-25 Wh/kg in state-of-the-art LIC to 40-45 Wh/kg for SIC, doubling the power density and increasing the efficiency for each cycle. Improvement of the energy density and power density will require less SIC cells to be manufactured for a given application, and an increased efficiency will result in less electricity losses during the use phase.

Secondly, the SIC is provisionally expected to be more sustainable due to the replacement of graphite, copper, and lithium, which are found on EU's critical raw material list[7], with hard carbon, aluminium, and more abundant sodium, respectively. Particularly, copper has high impacts on both resource depletion, acidification potential, and human toxicity potential[16]. Due to the characteristics of its supply chain, the possibility of using aluminium as the anode current collector in the SIC is therefore anticipated to be more sustainable than using copper as required in LIC/LIB, despite aluminium being also on EU's critical raw materials list. Hard carbon as the anode active material for SIC is expected to have a potential for more sustainable production if organic waste material is used[3], which will be investigated in MUSIC. Novel carbon materials from recycling processes will also be studied in MUSIC for potential applications in the anodes. Similarly, activated carbon can also be produced from organic waste materials, thereby not relying on limited resources. Activated carbon produced from sawdust will be used in MUSIC. A minor drawback of carbon materials such as hard carbon and activated carbon may be that they are relatively low-value materials, whereby it might not be economically feasible to recycle these materials after end-of-life without further research into novel recycling methods for these materials.

By mixing a pre-sodiation agent into the activated carbon slurry during manufacturing, an additional process step is avoided, whereby little additional energy is required during manufacturing. MUSIC will also aim to develop sustainable binders, both in terms of precursor materials but also by improving the electrode production process via development of dry methods or aqueous slurries that decrease the materials and energy demand. Sustainability aspects will also be considered during development of new electrolytes for the SIC cells to be produced in MUSIC.

In addition to the preliminary sustainability considerations described in this document, the MUSIC project will include a full LCA and economic analysis to assess the full potential of the SIC technology for selected applications. The analyses will follow the natural SIC cell and system development during MUSIC and include environmental and economic assessments of cell components at first, followed sequentially by first prototype, full device at industrial production, and system level including use case, second use, and recycling. The SIC cell and module development can thereby be supported and directed by the parallel LCA analyses performed, which is also preferably how research and development should be conducted by industry.

4 Recommendation

It is suggested that the general guidelines presented in this document are used by SIC manufacturers and module developers as a basis for a sustainable development of the SIC technology. In this way, sustainability aspects can be considered from the start of the technological development process, decreasing so the likelihood of spending large amounts of time and resources on technological pathways characterized with poor environmental performance. These guidelines should also be followed by the partners in the MUSIC project in terms of the cell and module specifications detailed in the deliverable.

As evidenced in the references attached, the focus on sustainability from governmental bodies and public and/or private collaborations/organizations is increasing, and several different regulations, guidelines, and standards are being developed worldwide. It is therefore highly recommended to follow these works, remaining up to date on their findings to quickly react and adapt the technology based on new legislations.

5 Risk register

Risk No.	**What is the risk**	**Probability of risk occurrence**[1]	**Effect of risk**[2]	**Solutions to overcome the risk**
WP2	The material selected for cell and module development do not have the lowest environmental impact.	Medium	Medium	Use phase has to compensate the higher efforts and impacts during the manufacturing process with the selected materials

Table 1: Risk Register

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[1] Probability risk will occur: 1 = high, 2 = medium, 3 = low

[2] Effect when risk occurs: 1 = high, 2 = medium, 3 = low

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Project partners

#	PARTICIPANT SHORT NAME	PARTNER ORGANISATION NAME	COUNTRY
1	CICE	CENTRO DE INVESTIGACION COOPERATIVA DE ENERGIAS ALTERNATIVAS FUNDACION, CIC ENERGIGUNE FUNDAZIOA	Spain
2	EUR	CLANCY HAUSSLER RITA	Austria
3	KIT	KARLSRUHER INSTITUT FUER TECHNOLOGIE	Germany
4	CNRS	CENTRE NATIONAL DE LA RECHERCHE SCIENTIFIQUE CNRS	France
4.1	IMN	NANTES UNIVERSITE (Affiliated)	France
5	UPS	UNIVERSITE PAUL SABATIER TOULOUSE III	France
6	FSU	FRIEDRICH-SCHILLER-UNIVERSITAT JENA	Germany
7	IRT-JV	INSTITUT DE RECHERCHE TECHNOLOGIQUE JULES VERNE	France
8	ELY	E-LYTE INNOVATIONS GMBH	Germany
9	BYD	BEYONDER AS	Norway
10	BCARE	BATTERYCARE S. L.	Spain
11	TALGO	PATENTES TALGO SL	Spain

Table 2: Project Partners

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