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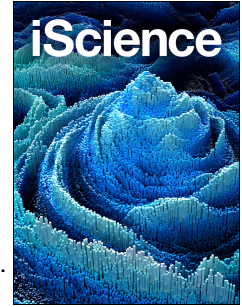
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# Journal Pre-proof



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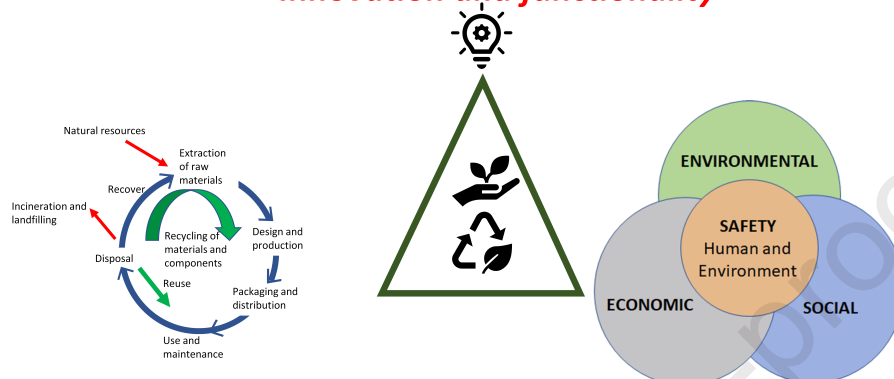
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## A holistic LCT SSbD Approach for battery technologies

**Step 1. Identification of criticality, toxicity, environmental, social, circularity, functionality and economic impacts following life cycle thinking principles**

Step 1: Identification of safety and sustainability issues	Life cycle stage				
	Raw materials and resources	Processing (material)	Manufacturing (product)	Use (product)	End-of-life (product)

### Innovation and functionality



### Life Cycle Thinking (LCT)

### Sustainability:

Including the new understanding of 'safety' according to the European Chemical Strategy for Sustainability

Criticality – are critical materials used?	Toxicity impact	Environmental impact	Social impact	Circularity impact	Functionality	Cost



**Step 2: Development of Safe-and-Sustainable-by-Design strategies using green chemistry and Circular Economy principles**

Step 2: Developing and communicating SSbD Strategies*						
	Raw materials and resources	Processing (material) Manufacturing (product)	Life cycle stage			Improvements in functionality (efficiency, durability)
			Use (product) End-of-life (product)	End-of-life (product)		
Battery technology	Re-think/ Re-Design	Remanufacture (material or product)	Recycle (material and product)	Replace or Reutilize (material and/or product)	Recover (material and/or product)	

**Step 3: Verification of Safe-and-Sustainable-by-Design strategies to ensure they lead to safer and more sustainable alternatives**

# **Life cycle thinking and safe-and-sustainable-by-design approaches for the battery innovation landscape**

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**Summary:**

Developments in battery technology are essential for the energy transition and need to follow the framework for Safe-and-Sustainable-by-Design (SSbD) materials, chemicals, products and processes as set by the EU. SSbD is a broad approach which ensures that chemicals/advanced materials/products/services are produced and used in a way to avoid harm to humans and the environment. Technical and policy-related literature was surveyed for battery technologies and recommendations were provided for a broad SSbD approach that remains firmly grounded in Life Cycle Thinking principles. The approach integrates functional performance and sustainability (safety, social, environmental and economic) aspects throughout the life cycle of materials, products and processes, and evaluates how their interactions reflect on SSbD parameters. 22 different types of batteries were analyzed in a life cycle thinking approach for criticality, toxicity/safety, environmental and social impact, circularity, functionality and cost to ensure battery innovation has a green and sustainable purpose to avoid unintended consequences.

## Abstract

Developments in battery technology are essential for the energy transition and need to follow the framework for the definition of Safe-and-Sustainable-by-Design (SSbD) criteria for SSbD chemicals and materials as set by the EU. SSbD is a broad approach which ensures that chemicals/advanced materials/products/services are produced and used in a way to avoid harm to humans and the environment. Here, technical and policy-related literature was surveyed for battery technologies and recommendations were provided for a broad SSbD approach that remains firmly grounded in Life Cycle Thinking principles. The approach integrates functional performance and sustainability (safety, social, environmental and economic) aspects throughout the life cycle of materials, products and processes, and evaluates how their interactions reflect on SSbD parameters. This review, and the proposed approach is conducted in two phases. Firstly, aspirations and targets are identified which are used to define relevant toxicity/safety, environmental, social, functionality and economic parameters for batteries, including a qualitative review of the current situation, an inventory of possible SSbD strategies that can be applied at the design stage to improve these parameters (i.e. green chemistry and circular economy), and an outlook for the battery innovation landscape in meeting these SSbD parameters. In the second phase, 22 different types of batteries (liquid & polymer gel, solid state, redox-flow and hybrid) were analyzed for criticality, toxicity/safety, environmental and social impact, circularity, functionality and cost. This analysis takes into account the big picture (life cycle thinking) to ensure battery innovation has a green and sustainable purpose to avoid unintended consequences.

**Keywords:** EU Chemical Strategy for Sustainability, social impact, environmental impact, safety, next generation batteries, unintended consequences

## Introduction: Transitioning towards a toxic-free environment to meet policy ambitions

Recent policy developments such as the European Green Deal [1-3], the European Chemical Strategy for Sustainability (EC-CSS) [4] and the Zero Pollution Action Plan [2] warrant the application of Life Cycle Thinking (LCT) principles [5] to meet policy ambitions. LCT is about including environmental, social and economic impacts of products and services over their entire life cycle and going beyond industrial production and manufacturing processes [6, 7]. LCT approaches include Life cycle Management, Environmental Life Cycle Assessment (LCA), Social Life Cycle Assessment (S-LCA), Life Cycle Costing (LCC), Life Cycle Sustainability Assessment (LCSA), carbon footprinting, and water footprinting [6]. The EC-CSS puts forth a new understanding of sustainability, safety and the applicability of safe-and-sustainable-by-design (SSbD). SSbD is a central element in the EC-CSS and here we explore how LCT principles can be adapted for the operationalization of SSbD.

In the EC-CSS, the ambitions towards a toxic-free environment and protection against the most harmful chemicals are evident. An important development is the extension of the generic approach to risk management to ensure that chemicals that cause cancers, gene mutations, affect the reproductive or the endocrine system, or are persistent and bioaccumulative are not present in consumer products. This generic approach will be extended to other harmful chemicals including those affecting the immune, neurological or respiratory systems and chemicals toxic to specific organs [4]. The commonly used LCA approach assess environmental impacts from chemical emissions from a human safety perspective (e.g., disability-adjusted life years or DALYs as an indicator), yet the new endpoints outlined in the EC-CSS such as endocrine disruption, neurotoxicity and specific organ toxicity are not specifically considered. LCA can only give an indication of potential total impacts, which does not reflect actual risk. For this reason, an integrated approach is warranted to address these ambitions as mentioned in the EC-CSS [4].

A first description of the SSbD concept can be found in the EC-CSS: “*safe-and-sustainable-by-design can be defined as a pre-market approach to chemicals that focuses on providing a function (or service), while avoiding volumes and chemical properties that may be harmful to human health or the environment, in particular groups of chemicals likely to be (eco) toxic, persistent, bio-accumulative or mobile. Overall sustainability should be ensured by minimizing the environmental footprint of chemicals in particular on climate change, resource use, ecosystems and biodiversity from a life cycle perspective*”[4]. Although in the EU-CCS, the SSbD concept is merely applied to chemicals, we believe it can be extended to include other materials and products as well.

The EC Joint Research Center (JRC) has developed a framework for SSbD criteria where a two-phase approach is recommended [8]. In the *(re)design phase*, SSbD principles have been identified by the EC JRC including: 1) *Material efficiency*, 2) *Minimizing the use of hazardous chemicals/materials*; 3) *Designing for energy efficiency*; 4) *Using renewable sources*; 5) *Preventing and avoiding hazardous emissions*; 6) *Reducing exposure to hazardous substances*; 7) *Designing for end-of-life*; and 8) *Consideration of the whole life cycle* [9]. In the *sustainability assessment phase*, five steps were provided for defining criteria for SSbD chemicals and materials [8].

## **A defining moment for batteries**

Assimilation of the SSbD and LCT principles is especially relevant at this time for batteries because of the exponential rate in innovation and their important role in energy transitions across the globe [10]. Current battery technologies such as lithium-ion face important challenges and research and development efforts are underway to develop so-called next generation batteries. Most of the recent advances in lithium-ion energy density have come from manipulating the relative quantities of cobalt, manganese and nickel in the cathode [11]. Cobalt is toxic, expensive, and deeply entrenched in unethical mining practices [12]. Nickel is not only toxic but the extraction of nickel, mainly mined in Australia, Canada, Indonesia, Russia and the Philippines, comes with environmental and health costs [13]. Nickel and cobalt are classified as carcinogenic and mutagenic materials, and this is also the case for toxic organic electrolytes which adversely affect human health and the environment [14]. Even though there are major safety and sustainability issues with nickel and cobalt, batteries dominating the market are expected to contain cobalt in some capacity in the coming years. For instance: in a lithium, cobalt, nickel, manganese oxide dominated battery, the demand is estimated to increase by factors of 18–20 for lithium, 17–19 for cobalt, 28–31 for nickel, from 2020 to 2050. This requires a drastic expansion of lithium, cobalt, and nickel supply chains, and likely also additional resource discovery [15, 16].

## **Aim of this review**

We surveyed technical and policy-related literature in relation to battery technology development and offer recommendations for a broad SSbD approach that remains firmly grounded in LCT principles. The approach integrates functional performance and sustainability (safety, social, environmental and economic) aspects throughout the life cycle of materials, products and processes, and evaluates how their interactions reflect on SSbD parameters. This review (and the proposed approach that emerges from it; Figure 1) is conducted in two phases. In the first phase we identify aspirations and targets which are used to define relevant SSbD parameters for batteries. Here, an overview of potential sustainability, and functional performance targets in support of the Green Deal [17], the EC-CSS [4] and other relevant policy documents was developed [9, 18]. Having identified these dimensions, The approach integrates functional performance and sustainability (safety, social, environmental and economic) aspects throughout the life cycle of materials, products and processes, and evaluates how their interactions reflect on SSbD parameters. We also explain how quantitative assessment tools such as LCA and S-LCA are used in practice to evaluate these dimensions. In the second phase, 22 different types of batteries (liquid & polymer gel, solid state, redox-flow and hybrid) were analyzed for criticality, toxicity/safety, environmental and social impact, circularity, functionality and cost. We finalize by discussing the challenges and opportunities, and provide recommendations for innovation in battery technologies keeping the big picture in mind to avoid blind spots by using a LCT-based SSbD approach to meet policy ambitions.

## **SSbD parameters in the policy and technological battery landscape**

### ***Survey of technical and SSbD ambitions for battery innovation***

Relevant SSbD parameters can be discerned at an early phase of the innovation process by identifying and operationalizing the sustainability (safety (risks concerning humans and the environment), environmental, social and/or economic impacts) issues and concerns that are

manifested. These issues can be linked to ambitions or targets that have been expressed in related policy documents. At the same time, it must be recognized that functional performance targets remain the key drivers of innovation, but they should be inextricably linked – positively and negatively- with safety and sustainability targets. The parameters that emerge from this survey can then be evaluated for each proposed battery design in order to identify opportunities to minimize potential hazard(s) and/or exposure [19] and to maximize sustainability.

### ***Functional performance parameters driving innovation***

From a functional performance perspective, there are several potential targets desired in batteries as proposed by Desjardins [20]: 1. High specific energy: referring to the total amount of energy stored by a battery; 2. High specific power: referring to the amount of load current drawn from the battery; Affordable cost: referring to the price of a particular battery type, in comparison to the current market value of comparable products; 4. Long life: referring to the number of charge/discharge cycles; 5. Wide operating range: referring to the range of temperatures where the battery can be functional; 6. Fast charging: referring to the time it takes for the battery to charge (optimum time for use); 7. Low self-discharge: referring to the amount of discharge when left alone without use over time; and 8. Long shelf life: referring to the longevity and shelf-life of the battery [20].

### ***SSbD parameters in the policy landscape***

The EC-CSS is part of EU's zero pollution ambition, which is a key commitment of the European Green Deal [4, 17]. The EC-CSS puts forth ambitions such as *'better protect citizens and the environment; boost innovation for safe and sustainable chemicals; SSbD chemicals, products and processes; non-toxic material cycles; the ban of endocrine disrupting chemicals in consumer products; the protection of humans and the environment against harmful chemicals; and avoiding chemical pollution in natural environments'*.

SSbD targets safety, environmental, social and economic sustainability dimensions of chemicals and products, which are also key commitments of the European Green Deal [17]. For safety, safe-by-design aspirations target *i) safer materials and products aiming to minimize, in the R&D phase, possible hazardous properties of the product while maintaining function; ii) safer production, ensuring industrial safety during the production of products, more specifically occupational, environmental and process safety aspects; and iii) safer use and end-of-life, minimizing exposure and associated adverse effects through the entire use life, recycling and disposal of the product. This can also support the transition towards a circular economy* [19, 21]. These targets are listed in Table 1. Circularity principles should be applied to safeguard sustainability in a product's life cycle. Potential impacts along a battery's life cycle should be considered in the design phase already (Eco-design), through re-thinking/re-designing materials or products. Simultaneously, resource-efficiency regarding (critical) raw materials should be considered in this stage of the life cycle. In the next life cycle stage, remanufacturing may help in achieving efficient use of water and energy; reduction of waste and emissions; and recovery of waste, water and energy. Finally, before the end-of-life stage products may be reused, and during end-of-life they should either be recycled or recovered. SSbD entails both the safety as well as the sustainability targets, which can be found for batteries in Table 1.

### ***Balancing functional performance and SSbD parameters***

Operational parameters that determine a battery's performance are directly tied to social and environmental impacts because performance in turn affects the total quantities of materials and energy that are consumed per unit of service offered by the battery (e.g., kWh delivered over the battery's lifetime). This only becomes evident when a life cycle approach is taken for a social and environmental impact assessment. Here several operational parameters are highlighted that are key to delivering the performance parameters while directly influencing the safety and sustainability of the battery over its life cycle.

Important functionality parameters include energy efficiency, Coulomb efficiency, power density and energy density, cycle life and shelf life, and electrolyte/electrode degradation (See Supplemental Material, Table 1 for descriptions).

When considering these aspects, it is important to take into account that performance parameters may influence each other, and thus may also indirectly influence the safety and sustainability of the battery. Furthermore, innovation strategies to improve performance may target battery chemistry/electrolyte, but also other battery components and ancillary systems. In SSbD, the former naturally gets the most attention as the electrolytes tend to represent a large percentage of the battery based on mass. The electrolyte is also where more specific demands are placed on material compositions, sometimes driving the need to resort to critical, expensive and/or potentially toxic materials. However, innovations in the latter category can improve the battery's performance, resulting in an optimization in the overall material and energy use throughout the life cycle of the batteries [16]. Recent innovations in industrial battery technologies are trying to adhere to SSbD, for instance by using lithium metal for battery anodes along with ceramics as the electrolytes to potentially double EV range for the same size battery while reducing safety hazards [22].

### **Evaluation of SSbD parameters in batteries**

#### ***Sustainability: Safety***

The safety of battery technologies can be evaluated by first making an inventory of the chemicals used in the different parts of the battery. Safety information can then be gathered from the following sources by filling in chemical name or preferably CAS number: 1. The Classification, Labelling and Packaging (CLP) inventory that is part of the Registration, Evaluation, Authorisation, and Restriction of Chemicals (REACH) regulation and that is available from the European Chemicals Agency website [23] 2. PubChem [24]; and/or search for Material Safety Data Sheets or Safety Data Sheets by googling 'safety data sheet' with the chemical name and CAS Number. In the ECHA Database, scroll to key data sets and click on 'C&L inventory' to find the toxicity information. In addition, an overview was made of whether the chemicals in batteries are in the list of Substances of Very High Concern (SVHC) [25-27]. A detailed inventory of safety aspects for the batteries evaluated is presented in the Supplemental Material.

#### ***Sustainability: Environmental***

Life cycle assessment (LCA) is a common method used to evaluate the environmental aspect of sustainability and it builds an inventory of all activities and the corresponding environmental emissions (as well as natural resource consumptions) that take place in the life

cycle of a product or service. These emissions/consumptions quantities are scaled to the amounts required to deliver a specific unit of product or service, i.e., the *functional unit* [28]. In the case of batteries, different functional units have been proposed (e.g., based on power capacity [kW], energy storage capacity [kWh], or delivery of stored energy [kWh]), making comparisons difficult [29-31]. The recent proposal for a EU batteries regulation prescribes the following definition: “*The functional unit is further defined as one kWh (kilowatt-hour) of the total energy provided over the service life by the battery system, measured in kWh. The total energy is obtained from the number of cycles multiplied by the amount of delivered energy over each cycle*”[32]. Other key aspects are yet to be standardized as well, such as system boundaries, e.g., how to include recycling and how/if to account for energy sources used to charge the batteries.

LCA then translates the total emissions/consumptions incurred in delivering the functional unit to a set of impact category indicators, e.g., climate change, ozone depletion, acidification, eutrophication, resource depletion and others [33]. Some LCA methods also include human toxicity and ecotoxicity indicators, which are closely related to the chemicals safety approaches already discussed. However, the LCA method is primarily challenged by the lack of emission and toxicity data. In their critical review of LCA impact assessment methods, the European Commission marked these categories with recommendation levels II/III; “recommended but in need of some improvements” and “recommended, but to be applied with caution”, respectively [34].

While quantifying the way in which material use can harm humans and ecosystems can be challenging for LCA, a more direct screening indicator for batteries is the intrinsic ecotoxicity of materials. Ecotoxicity can be determined with respect to many different endpoints. A common measure that can be used to compare battery materials is the predicted no-effect concentration (PNEC) or No Observable Effect level (NOEL), for which large databases have been made publicly available. Chemicals used in batteries had the following toxicity profiles: carcinogenicity, mutagenicity, reproductive toxicity, specific organ toxicity, endocrine disruption, respiratory sensitization, respiratory irritation, skin sensitization, skin corrosion, eye irritation, and/or aquatic toxicity.

#### *Environmental: resource use, critical materials and supply risks*

Criticality refers to limited reserves of minerals (geological and economically recoverable), together with different kinds of supply risk (e.g., technological, geopolitical). This aspect usually applies to metals and metalloids. Although criticality is a moving target and geographically dependent, a good reference is the EU Critical Materials list [35]. Graedel et al. [36] also offers a composite semi-quantitative indicator for metals and metalloids. The other side of the coin for criticality is abundance, which usually comes with cheaper prices and makes the use of non-metals and organic materials favorable in batteries. Criticality is a vital sustainability issue with battery technologies because there are supply risks for lithium, cobalt, graphite, vanadium, antimony, titanium, alloying elements, and cerium.

Criticality indicators can be produced following the EU methodology or that of Graedel et al. [36], which consider different factors. In the former, criticality is based on supply risk of the material (entailing: possible export restrictions, that increase supply risk or possible trade agreements, that decrease it; the bottlenecks in the whole material’s supply chain, not only the production stage; import dependency; and recycling, which may increase secondary supply and

thus reduce supply risk), and economic importance (assessed by allocating raw material uses to their corresponding economic sectors; and by taking into account the possible substitution of the materials, which may reduce economic importance) [37]. Graedel et al. [36] determine criticality based on supply risk (taking into account geological, technological, economic, social, regulatory and geopolitical indicators), environmental implications (defined by embodied energy and toxicity) and vulnerability to supply restriction (considering importance and substitutability on both a national and global level, and additionally taking into account susceptibility on a national level). This leads to a three-dimensional raw material ‘criticality space’.

### ***Sustainability: Social***

According to the draft EU Battery Regulation [38], identifying social risks associated with a battery’s supply chain will become compulsory for battery manufacturers in the near future. Addressing social aspects for life cycles is very challenging, since the social dimensions of the sustainability of batteries can be numerous and subject to a large degree of subjectivity in the choice of values and indicators. Social Life Cycle Assessment (S-LCA) attempts to overcome these barriers by combining quantitative and qualitative data and providing information on social and socio-economic aspects associated to all activities in the life cycle of one product or service. It is based on the same modeling principles as environmental LCA [39] and calculates impacts/risks on the basis of a functional unit.

An S-LCA can be conducted manually, which requires a lot of effort and detailed data. It can also be conducted with the help of databases such as the PSILCA database [40]. PSILCA was developed in compliance with the UNEP S-LCA guidelines and contains data for 19 subcategories and 65 qualitative and (semi-)quantitative indicators on social risks and impacts, covering around 15,000 country-specific industry sectors and commodities in 189 countries [39]. The database incorporates social indicators for different stakeholder groups, namely workers, local community, society, consumers and value chain actors. Data used in PSILCA comes from recognized sources such as ILOstat, World Bank, etc. [41]. For this analysis, the PSILCA database was used in OpenLCA (GreenDelta [42]). S-LCA databases such as PSILCA have a low resolution (country/sector level for minerals), but this allows them to be comprehensive and cover a wide range of impacts. In this way, S-LCA can be used as an initial guide to identify potential hotspots along the supply chain. It can be generalized that the majority of social impacts will most likely be traced back to mining of metals and metalloids [34]. Depending on the location and the type of mining that is required, different social risks may pose hotspots in the battery’s supply chain.

### ***Sustainability: Economic***

#### *Life cycle costing and levelized cost of storage (LCOS)*

Specific design choices can bring about economic benefits and losses, which are a fundamental part of the so-called triple-bottom line of sustainability. Life Cycle Costing is a well-accepted way to assess the economic dimension in the context of sustainability for three main reasons: it can account for externalities which are excluded from cost analysis, it considers the entire life cycle of the product or service, and it allows for cost accounting from the perspective of multiple actors in the value-chain, rather than one sole beneficiary such as the manufacturer [43]. Symeonidou et al. [44] developed a tool to conduct LCC for battery

energy storage systems integrated to residential PV installations. Bauman et al.[45] conducted an integrated LCC and CO<sub>2</sub> footprint evaluation of several battery types including Lithium-ion and Vanadium Redox-flow [43].

A more purely financial indicator is the Levelized Cost of Storage (LCOS) which can be defined as “*the minimum price per kWh that a potential investor requires in order to break even over the entire lifetime of the storage facility*” [46]. A well-known and often cited analysis of LCOS of different types of batteries is published periodically by Lazard [47]. LCOS is often used to optimize battery designs in terms of the functional performance parameters [46, 48]. However, this indicator is usually calculated for more mature systems such as Lithium-ion or Vanadium Redox Flow batteries [49, 50], rather than emerging designs that are still at pilot scale or earlier.

## **Battery innovation landscape in relation to technical and SSbD parameters**

### ***Overview of SSbD hotspots in the life cycle of battery technologies***

In light of the diverse -and often competing- sustainability parameters, each new innovation in battery design will have specific advantages and drawbacks. Here, key findings for liquid & polymer gel batteries, solid state and redox-flow batteries, and hybrid batteries focusing on each life cycle stage are discussed and summarized in Table 1 Overview of sustainability aspirations and targets for batteries

Table 2. A major result of the state-of-the-art overview is the realization that many of the substances used in new generation battery technologies are hazardous. Carcinogenic, mutagenic and/or reprotoxic chemicals are found in new generation battery technologies including cobalt, lithium carbon oxide, porous carbon, chromium and nickel. Copper is also under assessment for endocrine disruption. Chemicals that were toxic to aquatic life included antimony sulfide, zinc, vanadium, FL (viologen (4,4'-bipyridine derivative N-methyl-bipyridinium iodide), 9-fluorenone), TEMPO (quinone-based (1,2-benzoquinone-3,5-disulfonic acid), iron, chromium, bromine, (sodium) polysulfide, nickel, cerium, copper, chlorine and iodine. From a social perspective, it is not surprising that our findings showed that cobalt is associated with the highest social impact risks of the analyzed materials, as illustrated by the heatmap (Figure 2).

### ***Raw materials***

From a human and environmental impact perspective, nickel and cobalt are classified as carcinogenic and mutagenic materials, whereas organic electrolytes are not classified, yet safety data indicate these may adversely affect human health and the environment.

From an economic & criticality point of view, only a handful of countries generate almost all the world's lithium, creating an unstable commercial environment for stakeholders in this area. There is also the issue of supply and demand: global lithium reserves are not sufficient even to replace all cars in the world with electric vehicles (EVs), let alone provide batteries for the rest of the world's technology too [51, 52]. The limited supplies of rare and expensive elements like cobalt, manganese and nickel, which are found in the cathode materials of lithium-ion batteries are a cause for concern [51, 52]. On the other hand, on the 3 criticality scales proposed by Graedel et al. [36], none of the key materials in the current battery landscape rank high (70-100 score) except for lead (Pb), manganese (Mn) and chromium (Cr) on the

vulnerability to supply restriction scale, and cadmium (Cd) on the supply risk scale. We note, however, that this is based on a 2008 “epoch” and the methods and assumptions for a criticality assessment evolve quickly in time [36, 50].

With regard to social impact, two-third of the world’s cobalt, for example, comes from the Democratic Republic of Congo and about 20 % is estimated to come from sources that can be linked to unsafe working conditions and child labor [51-53]. ‘Conflict minerals’ such as tin, tungsten, tantalum and gold (also referred to as 3TG) are also of concern because their extraction and trade are usually in politically unstable areas, and can be used to finance armed groups, fuel forced labor and other human rights abuses, and support corruption and money laundering [54]. Figure 2 shows the S-LCA indicator scores for various raw materials present in the battery landscape. This offers a preliminary guidance for material selection based on social risks, as previous research suggests this is where most life cycle social risk hotspots are found [54-56]. In Figure 2 cobalt clearly ranks amongst the highest, however several aspects such as actual consumption, recovery, and country of origin of the material, must be considered to assess what these risks could mean for batteries in line with the LCT principles (see Supplemental Material, Box 1 – Social-LCA considerations for the case of cobalt).

### ***Battery production***

The potential human and environmental hotspots in cathode production and battery production include the emission of greenhouse gases in cell manufacturing and production of components for batteries (including the cathode, anode, current collectors, electrolyte, separator, and pouch materials) and in the manufacturing of cell components. Cell manufacturing is a key contributor accounting for 45 % of the greenhouse gases (GHG) emissions. The production and manufacture of materials and components for batteries account for 19 % of the GHG emissions. Additionally, cell manufacturing, cell components, and battery enclosure also dominate other pollutant emissions. Global Warming Potential (GWP) related to the release of Greenhouse Gases is also a problem from the common component package, battery management system (BMS), and energy (electricity and heat) demand, and from components of the battery including anode, anode binder, cathode, cathode binder, electrolyte, and separator [51, 52]. Note that the main drivers for GWP are the production of the cathode and cathode binder. For different Li-battery systems, discrepancies come from the cathode, because of the different mass shares of cathode current collector and cathode active materials [57].

Depending on the working conditions, social risks can also be incurred during manufacturing. A S-LCA of batteries for energy storage shows that manufacturing a battery in China entails higher social risks compared to a similar one in Germany, due to the difference in working conditions in the two countries [58]. Economic impacts for battery production are also expected [59].

### ***Operation***

Potential environmental hotspots during operation of batteries include energy losses during the charge/discharge cycles, with corresponding impacts linked to the original energy source. E.g. a less efficient battery charged from a coal source will have a high penalty [57]. Certain battery designs may increase or decrease parasitic energy loads on the whole system, e.g., the inability to operate efficiently at higher ambient temperatures may require cooling systems, reducing the overall efficiency.

For SSbD, the released chemicals from batteries are of importance because they imply safety risks to humans that are exposed to them [60] and to the environment. Other physical safety issues may arise from the operation and to the wider environment when the materials are released throughout the life cycle of the battery. The former case usually regards materials that cannot guarantee thermal stability, leading to combustion, fire, or explosion risks. During the operational phase, other materials such as halogens may lead to toxic gas emissions that require in-situ sequestration and careful monitoring. On a larger scale, released chemicals may also imply safety risks to humans that are exposed to them. Examples of safety issues during operation include the fire/explosion hazard of lithium-air batteries [61-64] or the thermal stability issues may lead to combustion, fire or explosion risks in lithium-iodine batteries [65-70].

### ***End-of-life***

There are many potential safety, environmental, social and economic hotspots. Major safety hotspots include hazardous chemicals in batteries and exposure to hazardous substances in waste. In lieu of well-developed recycling methods, often only a simple incineration or landfill treatment is considered in the assessments and in real life. An exponential increase in retired lithium-ion batteries in EV is expected up till 2050. The most generous reports suggest that currently 50 % of Li-ion batteries reaching the end of their life are recycled. The problem of recovery of essential materials such as Lithium is that the amount recovered is often too low to be suitable for reusability [57]. Major environmental impacts of recycling processes include landfill of waste material, incineration, and consumption of electricity, particularly for energy-intensive smelting processes. Informal and substandard recycling of batteries by children is a major social hotspot and also a leading contributor to poisonings such as lead poisoning in children living in low and middle-income countries [71]. Economic impacts include the costs associated with end-of-life.

### **Methodology in practice: Hybrid energy storage systems as a case study**

Hybrid energy storage systems use different energy storage technologies and have shown improvements in their technical performance and environmental sustainability [72]. In the selected case study, techno-hybridizations of four 1<sup>st</sup> and 2<sup>nd</sup> life battery technologies; Lithium Titanate (LTO), Lead-acid, Lithium Iron Phosphate (LFP) and Sodium-ion were compared with batteries for electric battery vehicles [72]. Table 3 shows the potential social risks, as well as the environmental impact categories as assessed by Koh *et al.* 2021 [72]. The application of SSbD strategies should be communicated as illustrated in Table 1 Overview of sustainability aspirations and targets for batteries

Table 2. Summary of sustainability and functionality/cost in state of the art battery technologies.

Table 3. Overview of safety, sustainability and functionality/ for hybrid energy storage systems as illustrative case study for SSbD applicability. Environmental impacts considered included environmental impact category; Global Warming Potential (GWP), Fossil Depletion Potential (FDP), Marine Eutrophication Potential (MEP), Freshwater Eutrophication Potential (FEP), Human Toxicity Potential (HTP) [72].

Table 4. Here the LTO/LTO/BEV is the hybrid energy storage system with the lowest environmental impact and thus was considered as a SSbD option in the illustrative case study.

## Conclusions and outlook

The main finding with respect to the literature review was that a LCT approach is necessary for applying and assessing SSbD strategies which have an impact. To the best of our knowledge, this is the first study that compares criticality, human toxicity, environmental toxicity, social impact, circularity, functionality and cost simultaneously for battery technologies. In addition, the currently applied LCT SSbD approach allows for transparency of which aspects have been addressed by SSbD and which aspects still need to be worked on. Creating safe and sustainable batteries is challenging because in addition to a holistic LCT SSbD approach, a value chain network is needed to ensure that safe and sustainable products are produced and used, whilst ensuring that sustainable value from the batteries is recaptured after use. Connecting the different stakeholders in the value chain and combining different disciplines is necessary to ensure that SSbD can be applied in practice. An organizational infrastructure is therefore needed to connect material scientists, human and environmental toxicologists, and sustainability experts with value chain personnel.

The potential sources of error in this analysis include uncertainties in the S-LCA and the use of secondary data for the environmental risk assessment. The underlying assumptions and uncertainties can be improved by performing a full LCA and environmental risk assessment and not relying on secondary data. An additional factor for consideration for policy makers and politicians is geopolitical impact to avoid blind spots including the exponential demand curve in the green energy transition. For instance, taking lithium which is a key component for batteries as a proxy, the global production has already increased by just short of 300% between 2010 and 2020 for direct lithium extraction [73]. The International Energy Agency reports that the current level of innovation, an electric car requires 6-times more mineral inputs than a conventional car [74]. The World Bank reports that current projections indicate that global production for minerals such as graphite and cobalt will increase by 500% by 2050, only to meet the demand for clean energy technologies [75]. Extra attention is needed to the socio-demographic problem of rare earths used in batteries. For the most part, these are mined in Africa, Latin America, Central Asia and in the Indo-Pacific, which are continents that not only need economic resources to accelerate their development pathway and climate adaptation but also have very real overlapping risk profiles. Geopolitical power is also a factor for consideration. The access to and processing of energy literally materializes into the ability to shape geopolitical power dynamics. China has skillfully leveraged its geo-economic rise to power over the last two decades on the back of integrating supply chains for rare earths from extraction to processing to export. China dominates the processing of lithium, nickel, cobalt and rare earths while their principle extraction is in Chile and Australia for lithium, Democratic Republic of Congo for cobalt, Indonesia and Philippines for nickel, and China for rare earths [74]. Finally, a fact that cannot be ignored is that the European Union is 98% dependent on China for rare earths putting China in a prime position to redesign the global balance of power [76].

This analysis and most important observation is that we can't just switch from one energy system, technology and/or material to another overnight without paying attention to the unintended consequences and the big picture. For industry, policy makers and politicians in Europe and in other countries, this review provides a transparent approach for assessing sustainability which applies a LCT and value chain perspective to avoid these blind spots. Future work should be aimed at reducing the need for energy and for critical materials which

starts with massive public and private investments into circular economic models that favor recyclability and material substitution. Future work should also be directed to integrate safety, social, economic and environmental assessments for supply chains that account for safety, social and economic impacts and environmental assessment including greenhouse gas emissions, and water, soil, biodiversity, material, and energy footprint. An integrated approach for safety assessment, LCA, S-LCA and life cycle costs is vital for applying SSbD. Safety assessment should include the new classification, labelling and packaging (CLP) hazard classes in REACH for: endocrine disruption; persistent, bioaccumulative and toxic (PBT); very persistent and very bioaccumulative (vPvB); persistent, mobile and toxic ('PMT'); or very persistent and very mobile (vPvM) [77]. It is imperative that next generation battery technologies implement a 'by-design' approach and not just a safety and sustainability assessment in order to try to avoid the use of critical materials, hazardous substances, production processes with high GHG and GWP and ensuring circularity and recyclability by avoiding landfill of waste material, incineration of plastics and energy-intensive smelting processes. LCA research needs to go beyond cradle to grave and demand industrial recycling data and avoid defaults such as using a simple incineration or landfill treatment. Further, an LCT approach takes into account the entire supply and distribution chains in order to ensure global transformation. The practical use of the holistic LCT SSbD approach as proposed in Table 1 Overview of sustainability aspirations and targets for batteries

Table 2. Summary of sustainability and functionality/cost in state of the art battery technologies.

Table 3. Overview of safety, sustainability and functionality/ for hybrid energy storage systems as illustrative case study for SSbD applicability. Environmental impacts considered included environmental impact category; Global Warming Potential (GWP), Fossil Depletion Potential (FDP), Marine Eutrophication Potential (MEP), Freshwater Eutrophication Potential (FEP), Human Toxicity Potential (HTP) [72].

Table 4 will not only ensure transparency of the SSbD applied strategies but also identify gaps in knowledge and identify aspects that were not taken into account. Overall, battery technology innovation needs to start shifting to bringing back economic footprint within planetary boundaries, and to having a green and sustainability purpose to avoid unintended consequences. The practical implications of this work for international policy makers in terms of regulation/standards, applications, and policy targets is to always keep the big picture in mind and the proposed holistic LCT approach can aid in this. For industry our analysis and review can be used as a basis and pragmatic guideline on how to integrate and optimize all aspects of sustainability (safety, environmental, social and economic impacts) and innovation in battery technologies. The data collected for the environmental risk assessment and human hazard classification can serve as a tool for industry for checking the hazards associated with the different battery components. This review also provides the databases available to perform these searches.

SSbD is an important component of the EC-CSS [4] and it is a broad approach aimed to ensure that chemicals/products/services are produced and used in a way that maximises their contribution to society while avoiding harm to the planet and future generations. In this review, an LCT SSbD approach was presented to identify the safety, environmental, social and economic hotspots and then assessing their impacts in some of the next generation battery technologies. A first attempt was made to integrate social aspects, in addition to functionality,

safety, human and environmental impacts towards a holistic approach. From a safety perspective, many of the substances used in battery technologies were found to be toxic, having carcinogenic, mutagenic and reproductive toxic properties, with few substances under assessment for endocrine disrupting properties (e.g. copper). SSbD strategies need to be directed at minimizing or eliminating the use of hazardous substances in battery technologies. From a sustainability perspective, environmental impacts (ecotoxicity of chemicals used) and social impacts (use of critical materials, mining practices) need to be addressed. From a performance and cost perspective, a balance between functionality and costs remains challenging. Here, approaches such as Multicriteria Decision Analysis might be useful in weighing economic, environmental, technological, and social dimensions for SSbD applicability and in selecting multi-dimension optimization [78, 79]. A general guidance for applying an LCT SSbD approach is provided in Figure 3.

A major challenge for the operationalization of SSbD is the lack of toxicity and LCA data at the early stage of the innovation process. In order to ensure maximum knowledge valorization, generating and connecting knowledge-based systems is needed to ensure synergies with ongoing knowledge generating initiatives, generating new knowledge and through cooperation as driver for knowledge building. This process should be coherent integrating not only disciplines (innovation, safety, sustainability, circularity) but also various stakeholders (industry, policy, academia and society) across the value chain and life cycles. Optimal use is needed of the full data-space on adverse effects. The basis for innovation and substitution should be that for every (new) chemical/material, a similarity comparison should be made with the full spectrum of 'like' substances (QSARs and read-across) to assess the expected potential to cause negative impact. In addition, methods assessing the uncertainty due to lack of data need to be further developed. For novel materials and novel battery technologies, a complete toxicity and sustainability profile is not expected. In this situation, a start screening for so-called 'risk and sustainability potentials' [80] can be performed in this first phase of design and battery development. Additional information about the novel materials has to be generated with the technology development of the battery. Here, a stage-gate approach can be applied to identify safety and sustainability information needs as potentials, indicators and demonstrators during the early, mid and late phase of the innovation process [19, 21, 80]. These issues and other industrial challenges should be addressed in ongoing initiatives such as BATTERY 2030+ [81] and the European Battery Alliance (EBA250 [82]) to stimulate innovation toward safe-and-sustainable chemicals in battery technology. This holistic LCT SSbD approach needs to be supported by a collaborative network involving the entire value chain for efficient knowledge sharing. Finally, this holistic LCT SSbD approach can guide battery innovators to keep the big picture in mind and in the practical implementation of SSbD in next generation batteries to meet international and EU policy ambitions.

### **Author contributions**

Willie Peijnenburg, Carlos Felipe Blanco and Lya G. Soeteman-Hernández conceived and led the research. Lya G. Soeteman-Hernández, Willie Peijnenburg and Carlos Felipe Blanco designed the paper. Carlos Felipe Blanco and Maarten Koese gathered information on the next generation batteries and conducted the S-LCA. Lya G. Soeteman-Hernández, Willie Peijnenburg and Carlos Felipe Blanco drew the discussion and wrote the paper with input from all coauthors. Adrienne J.A.M. Sips, Cornelle W. Noorlander provided consultations on the Life Cycle Thinking approach, as well as analysis, and reviewed the paper. All authors discussed the results and implications and contributed to the revision of the paper.

### **Credit author statement**

Lya G. Soeteman-Hernández: Conceptualization, Funding acquisition, Methodology, Writing - Review & Editing, Supervision; Carlos Felipe Blanco: Conceptualization, Investigation, Formal Analysis, Methodology, Writing - Review & Editing; Maarten Koese: Investigation, Formal Analysis; Adrienne J.A.M. Sips: Writing - Review & Editing, Cornelle W. Noorlander: Writing - Review & Editing; Willie Peijnenburg: Conceptualization, Funding acquisition, Methodology, Writing - Review & Editing, Supervision.

### **Data and materials availability**

All data needed to evaluate the conclusions in the paper are present in the paper. Additional data related to this paper may be requested from the authors.

### **Supplemental Material**

Supplemental material is provided and includes the following tables: Table 1 Important functionality parameters; Box 1 – Social-LCA considerations for the case of cobalt; Table 2 Overview of the toxicity of different components in batteries; Table 3 Safety, sustainability and performance/cost overview for liquid & polymer gel batteries; Table 4 Safety, sustainability and performance/cost overview for solid state and redox-flow batteries; Table 5 Safety, sustainability and performance/cost overview for hybrid batteries; Table 6 Extensive overview of safety, sustainability and performance parameters for liquid & polymer gel batteries; Table 7 Extensive overview of safety, sustainability and performance parameters for solid state and redox-flow batteries; Table 8 Extensive overview of safety, sustainability and performance parameters for hybrid batteries; and Table 9 Strategies for SSbD-driven innovation.

### **Declaration of competing interests**

The authors declare no competing interests.

### **Inclusion and diversity**

We support inclusive, diverse and equitable conduct of research.

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## Figure legends

Figure 1 A holistic Life Cycle Thinking SSbD approach integrating Life Cycle Thinking with sustainability and safety and with innovation and functionality (Step 1) for safe-and-sustainable-by-design applicability (Step 2). In the first step, sustainability issues are identified using Life Cycle Thinking principles. Here, criticality, toxicity, environmental, social, circularity and functionality impacts are identified. In the second step, SSbD strategies are applied using green chemistry and Circular Economy principles. It is important to note that every SSbD strategy needs to be verified to ensure they lead to safer and more sustainable alternatives (Step 3). \*For general SSbD driven innovation strategies, see Table 9 in the Supplemental Material.

Figure 2 Heatmap of the potential social risks related to the extraction of the different raw materials present in batteries, with increasing social impact from blue to red on the right-hand color heatmap indicator. Risks are expressed in “medium risk hours” (refer to PSILCA documentation) are normalized in this figure taking 1 kg of Lithium as a reference. Risks are evaluated for extraction in the country with the largest share of the global market.

Figure 3 LCT SSbD Guidance with ambitions and considerations. It is important to note that for the innovation and functionality aspect, batteries are not always on the same playing field and aspects such as marketing, media attention, social uptake, and most importantly funding (nationally, internationally, business viability) are very important. For instance, the batteries being used in EVs are standard, and this innovation market is hard to penetrate. Therefore, policy incentives are needed to stimulate the market entry of next generation battery technologies to stimulate SSbD in entrepreneurship practices and in the development of SSbD supportive business models. SVHC, Substance of very high concern [26, 27]; CMR, carcinogenic, mutagenic and reprotoxic chemicals; ED, endocrine disruptor (see list: [83, 84]); PBT, Persistent bioaccumulative toxic substances (see lists: [85-87]); PMT, Persistent, mobile and toxic [88]. For social impact determination, see Psilica.net [89]. For LCA datasets, see: OpenLCANexus [90].

## Table legends

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Table 4. The holistic Life Cycle Thinking SSbD approach in practice: Illustration on how to develop and communicate SSbD strategies

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Table 1 Overview of sustainability aspirations and targets for batteries

Aspect	Issue	Target/Aspiration	Source
<b>Safety</b>	Hazardous materials / products	Avoid the use of substances of very high concern (SVHC) and hazardous chemicals that cause cancer, gene mutations, affect the reproductive or the endocrine system, or are persistent and bioaccumulative; also including chemicals affecting the immune, neurological or respiratory systems and chemicals toxic to a specific organ.	REACH Directive (2006) [30] EU Chemicals Strategy for Sustainability (2020) [4]
		Ensuring industrial safety during production, more specifically occupational, environmental and process safety aspects.	
		Minimizing exposure and associated adverse effects through the entire use life, recycling and disposal	
<b>Environmental</b>	Reducing environmental impacts throughout all stages of the battery life cycle.	The use of the recycled material to clearly defined applications where there is no negative impact on consumer health and the environment, and where the use of recycled material compared to virgin material is justified on the basis of a case-by-case analysis	EU Chemicals Strategy for Sustainability (2020) [4]
		Using materials with the lowest possible environmental impact	EU Green Deal (2019) [10] Batteries 2030+ Roadmap (2020) [31]
		A supply chain due diligence policy should be implemented by the economic operator that places a battery on the EU market	EU Battery Regulation proposal (2020) [32]
		Design products in a way to optimize their environmental performance (Ecodesign)	Ecodesign Directive (2009) [33] Sustainable Products Initiative proposal (2022) [3]
<b>Social</b>	Reducing social impacts throughout all stages of the battery life cycle.	Using responsibly and sustainably sourced materials	EU Chemicals Strategy for Sustainability (2020) [4] EU Battery Regulation proposal (2020) [32]
		Using materials obtained in full respect of human rights as well as social and environmental standards	EU Battery Regulation proposal (2020) [32]
		A supply chain due diligence policy should be implemented by the economic operator that places a battery on the EU market	EU Battery Regulation proposal (2020) [32]
<b>Economic</b>	Critical materials / supply risk	Minimize depletion of critical raw materials	EU Green Deal (2019) [10] EU fourth list of critical raw materials (2020) [34] Report on Critical Raw Materials for Strategic Technologies and Sectors in the EU (2020) [35]
		Resource-efficiency	At the end of their life, batteries need to be collected, repurposed, remanufactured or recycled (in this order of preference for a sustainability point of view), feeding valuable materials back into the economy
		Meet recyclability targets (minimum content of recycled materials, carbon footprint, performance and durability and labelling, as well as meeting collection and recycling target	Batteries 2030+ Roadmap (2020) [31] EU Battery Regulation Proposal (2020) [32]

(improvement of the current figure of 45% collection rate to 65% in 2025 and 70% in 2030 while other batteries – industrial, automotive or electric vehicle ones – have to be collected in full)

Using materials that are recycled with high levels of recovery, in particular valuable materials such as cobalt, lithium, nickel and lead

EU Battery Regulation proposal (2020) [32]

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Table 2. Summary of sustainability and functionality/cost in state of the art battery technologies.

Battery Type	Criticality – are critical materials used?	Safety	Environmental impact	Social impact	Circularity	Functionality	Cost	Other drawbacks
<b>Liquid &amp; polymer gel batteries</b>								
Lithium-ion (benchmark) [72-79]	Supply risks of lithium, cobalt and graphite. Nickel is being monitored for inclusion by EU	+++	Impacts of lithium and cobalt mining	Impacts and risks of Cobalt mining in Congo. Lithium in Atacama (Chile, Bolivia)	Energy intensive recycling	Good energy & power density. High energy efficiency and cycle life	High cost of cobalt	Difficult to scale to larger devices
Sodium-ion [80-85]	Vanadium, lithium or antimony in cathode, titanium in anode	+++	May cause long lasting harmful effects to aquatic life	Moderate impacts of mining	Low value of second-life materials which makes recycling too expensive	Can benefit from advances in Li-ion due to similarities.	Low cost and easily scalable	Low energy density
Potassium-ion [86-89]	Graphite	++	Impacts of potash mining	Minor impacts of mining	No information to be found	High energy density, fast charging rates. Can benefit from advances in Li-ion due to similarities.	Low cost	Structural degradation and short cycle life
Lithium-Sulphur [79, 90-92]	Lithium	++	Impacts of lithium mining	Detrimental impacts related to lithium mining in Atacama (Chile, Bolivia)	Energy intensive recycling	Lighter, cheaper, and more powerful than li-ion. High energy density, 5x that of Li-ion. Low cycle life.	Low cost	Volume expansion of up to 80%, causing mechanical stress. Unwanted reactions with electrolytes. Poor conductivity and poor stability at higher temperatures.
Zinc-air [62, 63, 93, 94]	No	+++	Very toxic to aquatic life with long lasting harmful effects	Minor impacts of mining	Energy intensive recycling	High energy density, long operating life	Low cost	Irreversibility of zinc due to formation of dendrites and passivation.
Aluminum-air [62, 94, 95]	No	+	Impacts of aluminum mining	Minor impacts of mining	Aluminum can be recovered from electrolyte	High energy density, light weight	Low cost	Degradation due to reaction with hydrogen or formation of Al(OH) <sub>3</sub> or Al <sub>2</sub> O <sub>3</sub> on Al surface

Battery Type	Criticality – are critical materials used?	Safety	Environmental impact	Social impact	Circularity	Functionality	Cost	Other drawbacks
Lithium-Air [62-65, 79]	Lithium	+++	Impacts of lithium mining	Detrimental impacts related to lithium mining in Atacama (Chile, Bolivia)	Energy intensive recycling	High energy and power density; Low energy efficiency and cycle life	Low cost	Air is not pure enough and would need to be filtered. Lithium and oxygen form peroxide films that produce a barrier, ultimately killing storage capacity. Prone to oxidative degradation from the formation of Li <sub>2</sub> CO <sub>3</sub> . Cycle life is only 50 cycles in lab tests.
<b>Solid state and redox-flow batteries</b> Solid State Lithium-lithium [96, 97]	Metals in oxide electrolytes (Ga, Ta, La, Li) and cathodes (Co, Li).	+++	Impacts of lithium mining	Detrimental impacts related to lithium mining in Atacama (Chile, Bolivia)	Energy intensive recycling	Energy densities slightly higher than Li-ion, higher efficiency, reduction in weight and volume compared to Li-ion	Low cost	High resistance at ambient temperatures, intricate design, relatively low power density, high costs, fast degradation of lithium based cathodes
Redox-Flow Vanadium [98-101]	Vanadium	+++	Environmental impacts of vanadium as a by-product of uranium ore mining  May cause long lasting harmful effects to aquatic life	Impacts of mining Vanadium	Recyclability of the vanadium electrolyte	Using vanadium ions in different oxidation states to store chemical potential energy at scale. Can be expanded simply by using larger electrolyte tanks, minimal cross-over issues	High costs due to vanadium	Poor energy-to-volume ratio. Very heavy; must be used in stationary applications
Redox-Flow Organic [101-105]	No	+++	May cause long lasting harmful effects to aquatic life	No mining needed which prevents social risks	Recyclability of materials	High power density, high coulomb efficiency, can be scaled up easily, relatively low electrolyte cost	Relatively low electrolyte costs	Low energy density, relatively low energy efficiency, electrolyte degradation
Redox-Flow Iron-chromium [101, 106-110]	No	+++	Very toxic to aquatic life	Moderate mining impacts of iron and chromium	Recyclability of materials	Low energy density	Can be scaled up easily	-

Battery Type	Criticality – are critical materials used?	Safety	Environmental impact	Social impact	Circularity	Functionality	Cost	Other drawbacks
Redox-Flow Bromine-polysulfide [101, 110, 111]	No	+++	Very toxic to aquatic life	Minor mining impacts of bromine	No information to be found	Energy efficiency seems relatively low, can be scaled up easily	Low cost	-
Redox-Flow Quinone-Bromine [112-114]	No	+++	Very toxic to aquatic life	Minor mining impacts of bromine	No information to be found	High energy density, can be scaled up easily	Low cost	Lower power density than Vanadium Redox Flow Battery
<b>Hybrid batteries</b>								
Zinc-Bromine [101, 115-118]	No	+++	Very toxic to aquatic life	Minor impacts of mining	Energy intensive recycling	High energy density, non-perishable, inherent chemical simplicity, high degree of electro-chemical reversibility at the electrodes, rapid and full-depth discharge	Low cost but High cost power because it must be periodically fully discharged,	Low energy efficiency, short cycle life
Zinc-Nickel [115, 118, 119]	No	+++	Very toxic to aquatic life	Minor impacts of mining of zinc and nickel	Energy intensive recycling	Does not require catalysts for reactions, high power density, fast charge/discharge capability, long cycle life	Competitive costs	Electrode degradation, zinc electrodeposition on the negative electrode
Zinc-Lead dioxide [115, 120]	No	+++	Very toxic to aquatic life	Minor impacts of mining of zinc and lead	Energy intensive recycling	Does not require catalysts for reactions	No information to be found	Zinc electrodeposition, which limits long-term operation
Zinc-Cerium [115, 118, 121, 122]	No	+++	Very toxic to aquatic life	Minor impacts of mining of zinc and cerium	Energy intensive recycling	Does not require catalysts for reactions; highest thermodynamic open-circuit cell voltage among all the currently studied aqueous redox flow batteries.	High costs	Electrolyte cross-mixing, zinc electrodeposition which limits long-term operation

Battery Type	Criticality – are critical materials used?	Safety	Environmental impact	Social impact	Circularity	Functionality	Cost	Other drawbacks
Zinc-Iron [115, 118, 123, 124]	No	+++	Very toxic to aquatic life	Minor impacts of mining of zinc, moderate mining impacts of iron	Energy intensive recycling	high energy density and high energy efficiency. Does not require catalysts for reactions.	Low-cost range	Zinc electrodeposition, which limits long-term operation
Zinc-Chlorine [101]	No	+++	Very toxic to aquatic life	Minor impacts of mining of zinc and chlorine	Energy intensive recycling	Does not require catalysts for reactions	No information to be found	Zinc electrodeposition, which limits long-term operation
Zinc-Iodine [115, 125-128]	No	+++	Very toxic to aquatic life with long lasting harmful effects	Minor impacts of mining of zinc and iodine	Energy intensive recycling	High energy density. Does not require catalysts for reactions, ease of fabrication	Low cost	Self-discharge leads to poor cycle life, zinc electrodeposition, which limits long-term operation
Zinc-Polymer [115, 129-131]	No	+++	Very toxic to aquatic life with long lasting harmful effects	Minor impacts of mining of zinc	Energy intensive recycling	Stability, improved electrode cycle life	Low cost	Zinc electro-deposition, which limits long-term operation, viscosity of the electrolyte, relatively low efficiency
Lithium-iodine [66-71]	Lithium	+++	Very toxic to aquatic life	Detrimental impacts related to lithium mining in Atacama (Chile, Bolivia)	Energy intensive recycling	High energy efficiency, high energy density, long term stability	Low cost	Self-discharge leads to poor cycle life, low coulombic efficiency, fast capacity deterioration

*\*Toxicity, +++, carcinogenic, mutagenic, reproductive toxic, endocrine disruptor, toxic to aquatic life; substance of very high concern; ++ all other toxicity endpoints ; + only physical hazards such as flammability and oxidizer; See Tables 2-8 in the Supplemental Material.*

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Table 3. Overview of safety, sustainability and functionality/ for hybrid energy storage systems as illustrative case study for SSbD applicability. Environmental impacts considered included environmental impact category; Global Warming Potential (GWP), Fossil Depletion Potential (FDP), Marine Eutrophication Potential (MEP), Freshwater Eutrophication Potential (FEP), Human Toxicity Potential (HTP) [142].

Battery type	Criticality – are critical materials used?	Toxicity impact	Environmental impact	Social impact	Circularity	Functionality	Cost	Other drawbacks
Lithium-ion (benchmark) [84-89]	Supply risks of lithium, cobalt and graphite. Nickel is being monitored for inclusion by EU.	+++	Impacts of lithium and cobalt mining	Impacts and risks of Cobalt mining in Congo. Lithium in Atacama (Chile, Bolivia)	Energy intensive recycling	Good energy & power density. High energy efficiency	High cost of cobalt	Difficult to scale to larger devices
100% Lithium Iron Phosphate (LFP) [142]	Supply risks of lithium.	- (high safety)	GWP – 18,044,642 kg CO <sub>2</sub> -eq FDP – 5,184,230 kg oil-eq MEP – 14,800 kg N-eq FEP – 5917 kg P-eq HTP – 5,582,791 kg 1,4-DCB-eq.	Impacts and risks of lithium mining in Atacama (Chile, Bolivia)	Energy intensive recycling. Hydrometallurgy involves leaching with sulphuric acid, neutralisation, the recovery of the required metals and wastewater treatment.	Long cycle life, high rate discharge and high temperature resistance  The cycle life of the LFP battery is assumed to be 2,500 cycles	High cost LFP BEV (683 £/kWh)	
Baseline configuration								
Lead-acid/ Lead-acid/BEV [142]	No	+++	Very toxic to aquatic life Ratio to baseline configuration GWP – 1.5 ↑ FDP – 1.5 ↑ MEP – 1.47 ↑ FEP – 1.62 ↑ HTP – 1.65 ↑	Minor impacts of mining of lead	Energy intensive recycling. Hydrometallurgy involves leaching with sulphuric acid, neutralisation, the recovery of the required metals and wastewater treatment.	Does not require catalysts for reactions  The cycle life of the Lead-acid battery is assumed to be 1,500 cycles	Lead-acid (221 and 110 £/kWh for 1 <sup>st</sup> and 2 <sup>nd</sup> life battery technology)	
Na-ion/ Na-ion/BEV [142], [90-94]	Vanadium, lithium or antimony in cathode, titanium in anode	+++	May cause long lasting harmful effects to aquatic life Ratio to baseline configuration GWP – 1.18 ↑ FDP – 1.17 ↑	Moderate impacts of mining	Low value of second-life materials which makes recycling too expensive.	Can benefit from advances in Li-ion due to similarities.  The cycle life of the Na-ion battery is	Low cost and easily scalable Na-ion (278 and 139 £/kWh for 1 <sup>st</sup> and 2 <sup>nd</sup> life battery technology)	Low energy density

Battery type	Criticality – are critical materials used?	Toxicity impact	Environmental impact	Social impact	Circularity	Functionality	Cost	Other drawbacks
LFP/LFP/BEV [142]	Supply risks of lithium.	- (high safety)	MEP – 1.17 ↑ FEP – 1.24 ↑ HTP – 1.27 ↑ Ratio to baseline configuration GWP – 1.02 ↑ FDP – 1.03 ↑ MEP – 1.02 ↑ FEP – 1.1 ↑ HTP – 1.13 ↑	Impacts and risks of lithium mining in Atacama (Chile, Bolivia)	Energy intensive recycling. Hydrometallurgy involves leaching with sulphuric acid, neutralisation, the recovery of the required metals and wastewater treatment.	assumed to be 2,000 cycles  The cycle life of the LFP battery is assumed to be 2,500 cycles	LFP (217 and 73 £/kWh for 1 <sup>st</sup> and 2 <sup>nd</sup> life battery technology)	
LTO/LTO/BEV [142]	Supply risks of lithium and titanium.	+	Ratio to baseline configuration GWP – 2.16 ↓ FDP – 2.16 ↓ MEP – 2.12 ↓ FEP – 1.86 ↓ HTP – 1.68 ↓	Impacts and risks of lithium mining in Atacama (Chile, Bolivia)	Energy intensive recycling. Hydrometallurgy involves leaching with sulphuric acid, neutralisation, the recovery of the required metals and wastewater treatment.	The cycle life of the LTO battery is assumed to be 18,000 cycles	33% lower compared to lead-acid batteries	

LFP, Lithium Iron Phosphate; LTO, Lithium Titanate; BEV, Battery electric vehicle; Na, sodium. DCB, 1,4 dichlorobenzene in Koh *et al.* 2021 [142].

\*Toxicity, +++, carcinogenic, mutagenic, reproductive toxic, endocrine disruptor, toxic to aquatic life; substance of very high concern; ++ all other toxicity endpoints ; + only physical hazards such as flammability and oxidizer; - According to the majority of notifications provided by companies to ECHA in CLP notifications no hazards have been classified  
Toxicity information: LFP, [Substance Information - ECHA \(europa.eu\)](#); Lead acid, Carcinogenic (Some data submitters indicate they consider this substance as Carcinogenic), Toxic to reproduction, substance of very high concern (SVHC), [Substance Information - ECHA \(europa.eu\)](#); [Brief Profile - ECHA \(europa.eu\)](#); LTO, [SDS-Lithium-Titanate.pdf \(tamceramics.com\)](#)

Table 4. The holistic LCT SSbD approach in practice: Illustration on how to develop and communicate SSbD strategies

Step 1: Identification of safety and sustainability issues/hotspots	Life cycle stage			
	Raw materials and resources	Processing (material) Manufacturing (product)	Use (product)	End-of-life (product)
Environmental impact	Limited supplies of rare and expensive elements like cobalt, manganese and nickel, which are found in the cathode materials of lithium ion batteries, are a cause for concern [60, 61].	Greenhouse gases (GHG) in cell manufacturing: In the production and manufacture of materials and components for batteries, including the cathode, anode, current collectors, electrolyte, separator, and pouch materials In cell manufacturing, cell components, and battery enclosure also dominate other pollutant emissions Global Warming Potential (GWP) from: A common component package, battery management system (BMS), and energy (electricity and heat) demand components of the battery including anode, anode binder, cathode, cathode binder, electrolyte, and separator Environmental impact Leaching of chemicals due to mining [60, 61, 71].		Recycling Most LCA research only includes cradle to grave assessments owing to a lack of industrial recycling data or technology in the early stages of study, excluding the recycling stage. Usually only a simple incineration or landfill treatment is considered An exponential increase in retired Lithium batteries (LIBs) is expected by 2050 given a typical 5-8 year service life of (LIBs) in an electric vehicle (EV). The most generous reports suggest that currently 50% of Li-ion batteries reaching the end of their life are recycled. Problem: recovery of essential material is low, and often too low to be suitable. Major environmental impacts of recycling processes are: - landfill of waste material, - incineration of plastics, and - consumption of electricity, particularly for energy-intensive smelting processes [61, 71].
Social impact	Two-thirds of the world's cobalt comes from the Democratic Republic of the Congo and about 20% is estimated to come from sources that can be linked to unsafe working conditions and child labor [60, 61].			
Safety – human and environmental impact	Nickel (Ni) and cobalt (Co), are classified as carcinogenic and mutagenic materials, as well as toxic organic electrolytes, which adversely affect human health and the environment [25].			
Economic impact	- Only a handful of countries generate almost all of the world's lithium creating an unstable commercial environment for stakeholders in this area. - Global lithium reserves are not sufficient for demands such as electric vehicles and other technologies [60, 61].			

Step 2: Developing and communicating SSbD Strategies						
	Life cycle stage					Improvements in functionality (efficiency, durability)
	Raw materials and resources	Processing (material) Manufacturing (product)	Use (product) End-of-life (product)	End-of-life (product)		
Battery technology	Re-think/ Re-Design	Remanufacture (material or product)	Recycle (material and product)	Replace or Reutilize (material and/or product)	Recover (material and/or product)	
<p>LTO/LTO/BEV 1st/2nd life batteries/ BEVs</p> <p>Hybrid energy storage system where different generation, storage, and consumption technologies are combined in a single system.</p> <p>Application: stationary storage system</p>	<p>Material – Yes Process - No</p> <p>Innovation aspect: Anode – Yes Cathode - Yes</p> <p>No change in Collectors, Electrolyte, or Separator pouch</p>	<p>Resource efficiency (water, energy, materials) Yes</p> <p>Reduction of waste and emissions Yes</p> <p>Recovery of waste, water and energy No</p>	<p>Recycling process: Partly as 1st and 2nd generation life batteries are used</p> <p>Recycling method (Hydrometallurgy) is still energy intensive</p>	<p>Yes Remanufacture of 1st life batteries to be implemented into a useful system</p>	<p>No</p>	<p>Long cycle life - Yes Affordable cost</p> <p>Not accounted for: High specific energy High specific power Wide operating range Fast charging Low self-discharge Long shelf life [28].</p>

LFP, Lithium Iron Phosphate; LTO, Lithium Titanate; BEV, Battery electric vehicle; Na, sodium.

**Highlights**

- Safe-and-Sustainable-by-Design (SSbD) is central to meet EU policy ambitions
- Technical and policy-related literature was surveyed for battery technologies
- A life cycle thinking-based SSbD approach was developed for battery technologies
- 22 battery types were assessed including all safety and sustainability dimensions
- The big picture is important to avoid blind spots and unintended consequences

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**Declaration of interests**

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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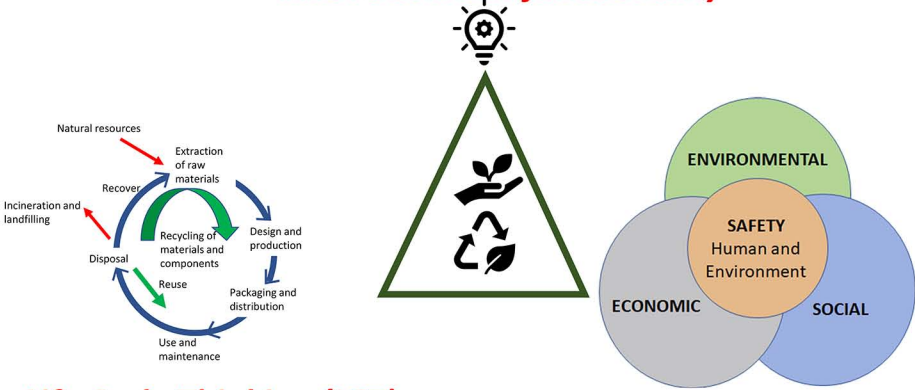
The authors declare the following financial interests/personal relationships which may be considered as potential competing interests:

# A holistic LCT SSbD Approach for battery technologies

**Step 1. Identification of criticality, toxicity, environmental, social, circularity, functionality and economic impacts following life cycle thinking principles**

Step 1: Identification of safety and sustainability issues	Life cycle stage				
	Raw materials and resources	Processing (material)	Manufacturing (product)	Use (product)	End-of-life (product)

## Innovation and functionality



## Life Cycle Thinking (LCT)

## Sustainability:

Including the new understanding of 'safety' according to the European Chemical Strategy for Sustainability

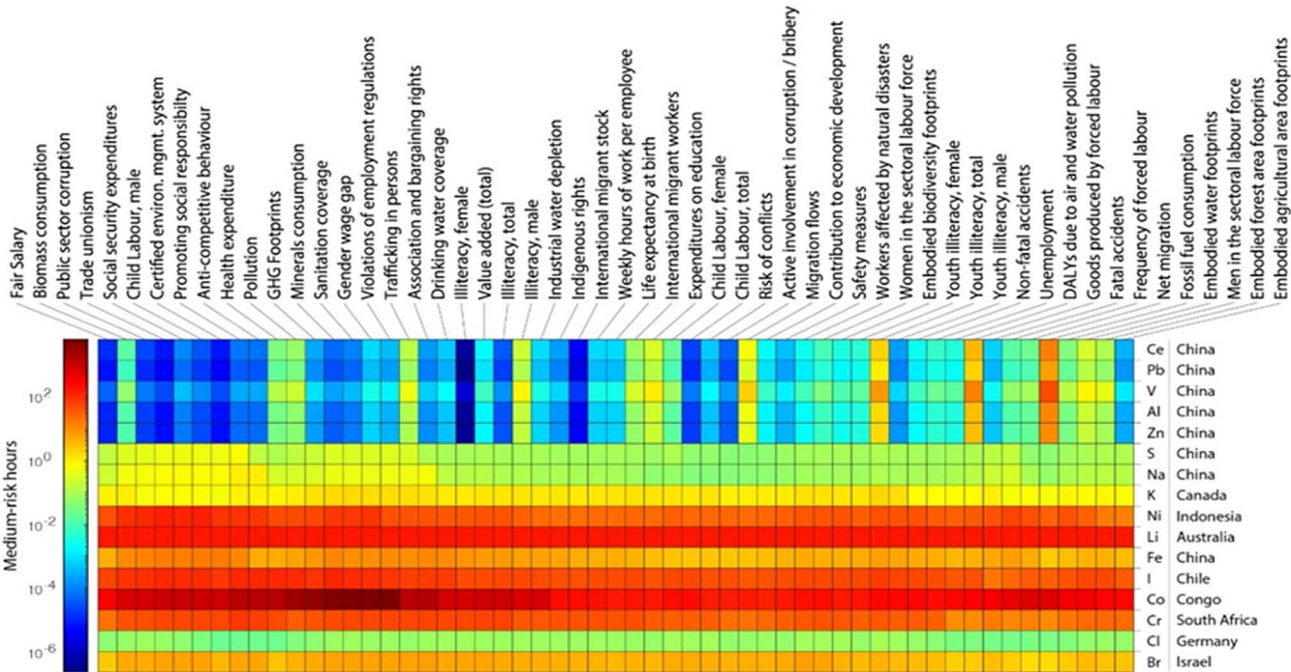
Criticality – are critical materials used?	Toxicity impact	Environmental impact	Social impact	Circularity impact	Functionality	Cost
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**Step 2: Development of Safe-and-Sustainable-by-Design strategies using green chemistry and Circular Economy principles**

Step 2: Developing and communicating SSbD Strategies*						
	Life cycle stage					Improvements in functionality (efficiency, durability)
	Raw materials and resources	Processing (material)	Use (product)	End-of-life (product)		
Battery technology	Re-think/ Re-Design	Remanufacture (material or product)	Recycle (material and product)	Replace or Reutilize (material and/or product)	Recover (material and/or product)	

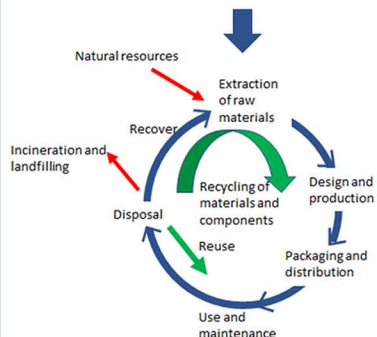
**Step 3: Verification of Safe-and-Sustainable-by-Design strategies to ensure they lead to safer and more sustainable alternatives**



**AMBITION: Maximize functionality and durability**

Functionality and cost: Does battery have a Long life, High specific energy, High specific power, Wide operating range, Fast charging, Low self-discharge, Long shelf life, and Affordable cost?

- Market entry factors: marketing, media attention, social uptake, and most importantly funding (nationally, internationally, business viability)
- On market or close to market?
- Scale of application?

**Innovation and functionality****AMBITION: Effective recyclability and reusability**

Safety: Are hazardous substances released during recycling?

Are efficient recycling processes available?

Environmental: Most LCA research only includes cradle to grave assessments owing to a lack of industrial recycling data or technology in the early stages of study, excluding the recycling stage.

Usually only a simple incineration or landfill treatment is considered.

Recovery problem: recovery of essential materials is low, and often too low to be suitable for reuse. Is there a high environmental footprint associated with recycling process?

Major environmental impacts of recycling processes for:

hydrometallurgical processes – effect on global warming via landfill

pyrometallurgical processes – effect on global warming is incineration of plastics

Mechanical and hydrometallurgical treatments can recover more materials with lower energy consumption than pyrometallurgical technology

Social: Are there social impacts such as informal and substandard recycling of batteries done by children?

**AMBITION: Safe and sustainable use**

Safety and sustainability: is the battery use-life safe and sustainable?

Functionality and Economic: Does the battery have a Long life, High specific energy, High specific power, Wide operating range, Fast charging, Low self-discharge, Long shelf life, and Affordable cost?

**AMBITION:**

- **Minimization of critical material use**
- **Minimization of energy, water, solvent and waste during raw material extraction**

Safety: Are raw material hazardous (SVHC, CMR, ED, PBT, PMT)? (i.e. nickel (Ni) and cobalt (Co), are classified as carcinogenic and mutagenic materials, as well as toxic organic electrolytes, which adversely affect human health and the environment)

Economic: Are critical materials used? Only a handful of countries generate almost all of the world's lithium creating an unstable commercial environment for stakeholders in this area. Global lithium reserves are not sufficient even to replace all cars in the world with EVs, let alone provide batteries for the rest of the world's technologies

Social: Are there any known socio-demographic impacts known about raw material extraction (i.e. child labor, poor labor conditions as with Cobalt)?

**AMBITION:**

- **Safe and sustainable production and distribution**
- **Reduction of global warming potential**
- **Minimization of energy, water, solvents and waste during design, production, packaging and distribution**
- **Reduction of environmental footprint**

Safety: Are there possible human or environmental hazards in the production process? (SVHC, CMR, ED, PBT, PMT)

Environmental: Battery production carries a large carbon footprint. Are significant greenhouse gases (GHS) expected in battery production?

GHG in cell manufacturing: In the production and manufacture of materials and components for batteries, including the cathode, anode, current collectors, electrolyte, separator, and pouch materials. In cell manufacturing, cell components, and battery enclosure also dominate other pollutant emissions. Is a large carbon footprint expected in battery production?

Is there Global Warming Potential (GWP) expected? High GWP is usually associated from the battery management system (BMS), and energy (electricity and heat) demand components of the battery including anode, anode binder, cathode, cathode binder, electrolyte, and separator.

Economic: what is the cost of upscaling, production, and waste disposal during production?

Social: Are there social impacts such as poor labor conditions?

Life cycle	Ambition	Considerations
Innovation & functionality	<b>Maximize functionality and durability</b>	Long life, High specific energy, High specific power, Wide operating range, Fast charging, Low self-discharge, Long shelf life, Affordable cost Market entry factors: marketing, media attention, social uptake, and most importantly funding (nationally, internationally, business viability)
Raw material extraction	<b>Minimization of critical material use</b>	Ensure raw materials are not in critical list
Design & production	<ul style="list-style-type: none"> <li>✓ <b>Safe and sustainable production</b></li> <li>✓ <b>Reduction of global warming potential</b></li> <li>✓ <b>Minimization of energy, water, and solvents</b></li> <li>✓ <b>Reduction of environmental footprint</b></li> </ul>	Minimize hazardous substances (check ECHA CLP; or Safety Data Sheet Information) Minimize energy, water and solvent use during design & production
Packaging & distribution	<ul style="list-style-type: none"> <li><b>Safe and sustainable packaging and distribution (transport)</b></li> <li><b>Minimize environmental footprint</b></li> </ul>	Minimize distance to deliver product or material Minimize energy, water and solvent use during packaging & distribution
Use & maintenance	<b>Safe and sustainable use</b>	Avoid hazardous substances during use Ensure durability and long-shelf life
End of life	<b>Effective recyclability and reusability</b>	Ensure effective recycling or reuse processes with maximum recovery of materials (closed materials and product loops)