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Life cycle assessment of emerging batteries

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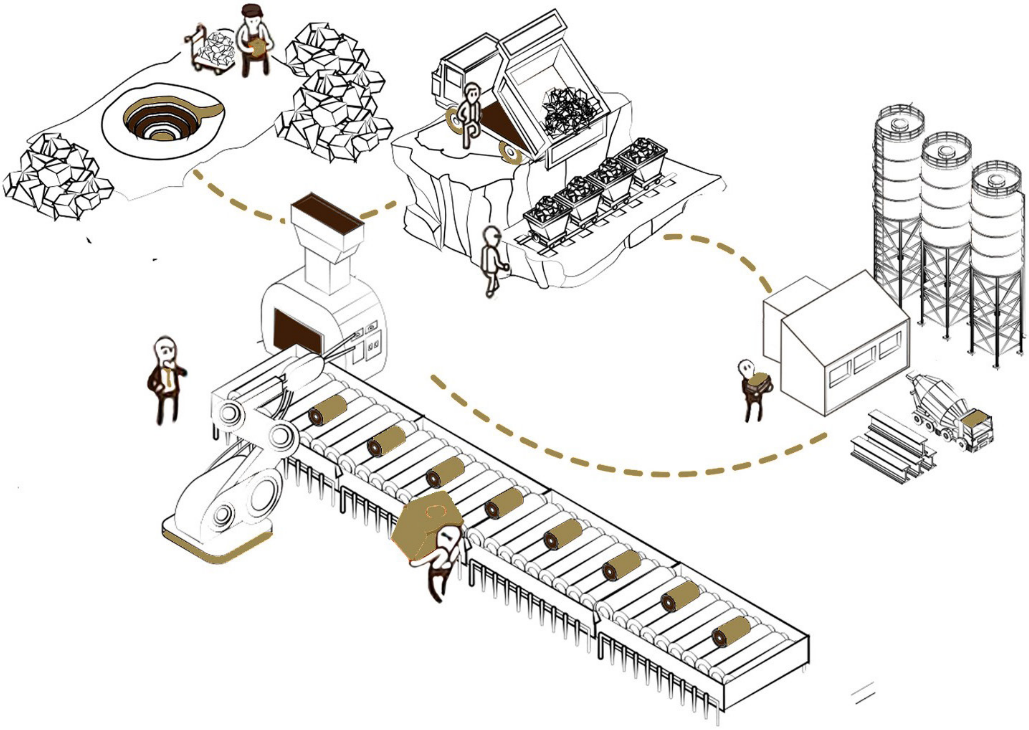

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Abstract

Population growth, economic development, and the transition to electrification are increasing the demand for advanced battery technologies, thus driving the development of next-generation batteries across various applications. This thesis explores the environmental impacts of emerging battery technologies: an all-organic battery, all-solid-state batteries (ASSBs), and sodium-ion batteries (SIBs) by life cycle assessment (LCA) and prospective LCA. Battery dimensioning models were developed to calculate material requirements and corresponding battery specific energy for ASSBs, SIBs and LIBs, ensuring comparability across different battery technologies.

Based on kWh battery capacity, the all-organic battery exhibits higher environmental impacts compared to the LIB, which is primarily due to its low energy density and the significant impacts associated with the electrode production. ASSBs show comparable or higher climate impact than LIBs, which mainly is due to the solid-state electrolyte and cathode active materials, with the anode and current collector being significant contributors in the polymer-based ASSB. Regarding SIBs, the layered oxide type has a climate impact comparable to LIBs, while the polyanion type and the preussian blue analogues type exhibit higher climate impact. Moreover, it was revealed that transitioning from laboratory-scale to large-scale production could significantly reduce the environmental impact, largely due to the optimized material use and solvent recycling. Indeed, studies on both ASSBs and SIBs highlight the significant potential for reducing climate impact through battery performance optimization and grid decarbonization. The results can help to guide development of more environmentally friendly battery technologies. Additionally, key methodological insights gained from the four studies are included.

Keywords: all-organic battery; sodium-ion battery; all-solid-state battery;
emerging technologies; prospective life cycle assessment; greenhouse gas
emission.

Livscykelanalys av nya batteritekniker

Sammanfattning

Befolkningsökning, ekonomisk utveckling och övergången till elektrifiering ökar efterfrågan på avancerade batteritekniker, vilket driver utvecklingen av nästa generations batterier för olika tillämpningar. Denna avhandling undersöker de miljömässiga effekterna av nya batteritekniker: ett helt organiskt batteri, fastfasbatterier (ASSB) och natriumjonbatterier (SIB) genom livscykelanalys (LCA) och prospectiv LCA (pLCA). Dimensioneringsmodeller utvecklades för att beräkna materielbehov och motsvarande energitäthet för ASSB SIB och litiumjonbatterier (LIB), vilket säkerställer jämförbarhet mellan batteriteknikerna.

Baserat på kWh batterikapacitet uppvisar det helt organiska batteriet högre miljöpåverkan jämfört med LIB, vilket främst beror på det organiska batteriets låga energitäthet och den betydande påverkan som är kopplad till elektrodproduktionen. ASSB visar jämförbar eller högre klimatpåverkan än LIB framförallt på grund av fastfaselektrolyten och katodaktiva material, där anoden och strömkollektorn är betydande bidragsgivare i polymerbaserade ASSB. När det gäller SIB har oxidtypen en klimatpåverkan som är jämförbar med LIB, medan polyanjon-typen och prussian blue analog-typen uppvisar högre klimatpåverkan. Dessutom påvisades att övergången från laboratorieproduktion till storskalig produktion skulle kunna minska miljöpåverkan avsevärt, främst på grund av optimerad materialanvändning och återvinning av lösningsmedel. Resultaten från studierna av ASSB och SIB visar på den stora potentialen att minska klimatpåverkan genom optimering av batteriprestanda och ökning av förnybar el i elnätet. Resultaten kan hjälpa till att vägleda utvecklingen av mer miljövänliga batteritekniker. Dessutom inkluderas viktiga metodologiska insikter från de fyra studierna.

Keywords: Organiskt batteri; Natriumjonbatteri; Solid state-batteri; Framväxande teknologier; Livscykelanalys; Prospektiv livscykelanalys; Växthusgasutsläpp

Dedication

To 21-year-old Shan

Contents

List of publications

This thesis is based on the work contained in the following papers, referred to by Roman numerals in the text:

I. Zhang, S., Ericsson, N., Hansson, P. A., Sjödin, M., & Nordberg, Å. (2022). Life cycle assessment of an all-organic battery: Hotspots and opportunities for improvement. Journal of Cleaner Production, 337, 130454.

II. Zhang, S., Ericsson, N., Sjödin, M., Potter, H. K., Hansson, P. A., & Nordberg, Å. (2022). Prospective life cycle assessment of a flexible all-organic battery. Journal of Cleaner Production, 337, 133804.

III. Zhang, S., Steubing, B., Potter, H. K., Hansson, P. A., & Nordberg, Å. (2024). Future climate impacts of sodium-ion batteries. Resources, Conservation and Recycling, 202, 107362.

IV. Zhang, S., Brandell, D., Valvo, M., Steubing, B., & Nordberg, Å. (2024) Future climate impact of all-solid-state batteries (submitted)

Papers I-III are reproduced with the permission of the publishers.

The contribution of Shan Zhang to the papers included in this thesis was as follows:

I. Planned the paper together with the co-authors. Performed data collection with inputs from co-author, modelling, and analysis. Wrote the paper with inputs from the co-authors.

II. Planned the paper with inputs from the co-authors. Performed data collection, modelling, and analysis. Wrote the paper with inputs from the co-authors.

III. Planned the paper. Performed data collection, modelling, and analysis. Wrote the paper with inputs from the co-authors.

IV. Planned the paper. Performed data collection with inputs from co-authors, modelling, and analysis. Wrote the paper with inputs from the co-authors.

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1. Introduction

Batteries have become essential components of contemporary life, powering applications ranging from portable electronics to electric vehicles (EVs) and stationary energy storage systems. As critical energy storage devices, batteries play a crucial role in both facilitating the transition towards a more sustainable society and enhancing energy security. Within the transport sector, transitioning from internal combustion engine vehicles to EVs can significantly reduce air pollution and greenhouse gas (GHG) emissions during the use phase of cars, and dependency on fossil fuels. To support this shift, several nations have implemented policies to promote EV sales (Yang et al., 2021b). Additionally, batteries enable the stable and flexible use of intermittent renewable energy sources in the energy system, therefore reducing the GHG emissions and the fossil fuels demand across various sectors (International Energy Agency, 2024a). Driven by factors such as population growth, economic development, and an accelerating global shift toward decarbonization, the demand for batteries is rapidly increasing (Yang et al., 2021b). In 2023, the usage of batteries in the energy sector exceeded 2400 gigawatt-hours (GWh), marking a fourfold increase since 2020. Over the past five years, more than 2000 GWh of lithium-ion battery capacity has been added, powering more than 40 million EVs and supporting thousands of battery storage projects (International Energy Agency, 2024a).

Currently, lithium-ion batteries (LIBs) dominate the market across different applications (Yang et al., 2021b). Each application has its own distinct requirements related to performance, user experience, cost, and safety. Current lithium-ion batteries often fall short in meeting all these diverse demands, which in turn encourages the exploration of alternative battery chemistries. Promising alternatives include organic batteries, non-lithium alkali-ion batteries such as sodium-ion batteries (SIBs), and all-solid-state batteries (ASSBs). Organic batteries employ metal-free, organic based electrode materials that could potentially be sourced from biomass, offering intrinsic bendability and flexibility that is ideal for some portable electronics (Hager et al., 2020). SIBs, which use abundant and low-cost sodium rather than lithium, offer an economical solution for short-range mobile and stationary energy storage applications (Tapia-Ruiz et al., 2021). ASSBs with solid electrolyte and pure lithium as anode are characterized by their high specific energy and enhanced safety, making them suitable for EVs (Schmaltz et al., 2022).

Despite the numerous conveniences that batteries bring to our lives, and their contribution to a more environmentally friendly future, the production of batteries also poses several environmental challenges. For instance, the extraction of battery minerals such as nickel, cobalt, and copper is often linked with high GHG emissions, significant toxicity impacts, acidification, eutrophication, and particulate matter (Farjana et al., 2019; Peters et al., 2017). Additionally, battery manufacturing processes are typically energy-intensive (Yuan et al., 2017). It is therefore crucial to evaluate the environmental impacts of emerging battery technologies during an early stage in their development when there is greater flexibility for modifications. Previous studies indicate that a significant portion of environmental impacts and associated costs are determined during the initial development phase (Thomassen et al., 2019). Early-stage environmental assessments provide stakeholders with valuable insights into the environmental performance of batteries. These findings can support the modification of input materials and production processes, therefore helping to minimize the adverse environmental consequences. These assessments can also identify and address data gaps, providing information for future studies. Life cycle assessment (LCA) is a widely used environmental assessment tool for quantifying the environmental performance of products and services, including battery technologies (Hauschild et al., 2018). Prospective LCA (pLCA) is particularly suited for emerging battery technologies, as it allows for the assessment of potential environmental impacts at a future point when these technologies are expected to be produced on a mass scale (Arvidsson et al., 2024).

2. Aim and structure

2.1 Aim and objectives

The overall aim of this thesis was to enhance our understanding of the environmental performance three different types of emerging battery technologies and to explore approaches for conducting life cycle assessments (LCAs) on these batteries. The batteries considered include an all-organic battery, two all-solid-state batteries, and three sodium-ion batteries. LCA and pLCA methodologies were used in the thesis. The specific objectives were as follows:

1). To quantify selected environmental impact categories associated with the life cycles of these batteries (Papers I-IV).

2). To identify environmental hotspots and provide recommendations for mitigating these impacts (paper I-IV).

3). To compare the environmental impacts of these emerging batteries with their lithium-based counterparts (paper II-IV).

4). To offer methodological guidance for conducting LCAs on emerging battery technologies, based on insights gained from paper I-IV.

2.2 Structure of research work

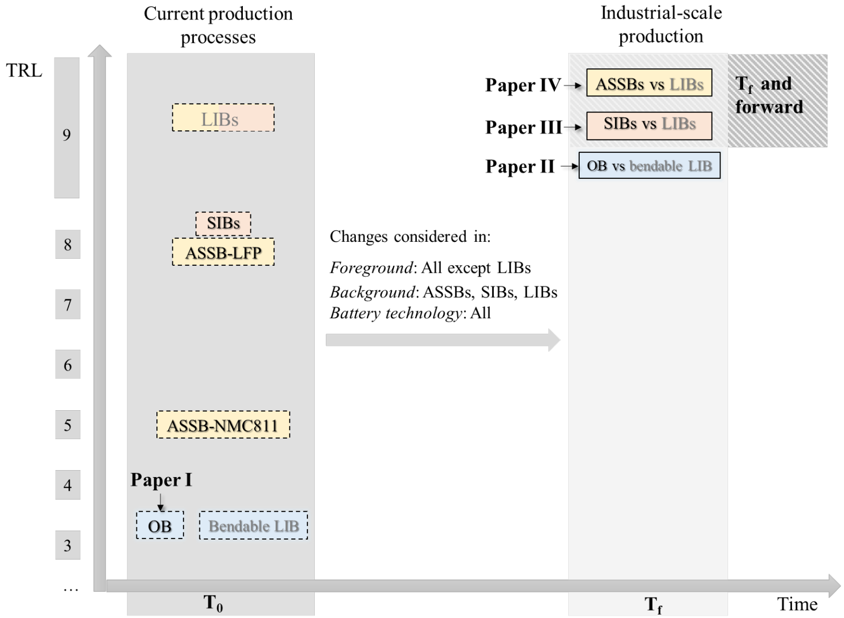

Figure 1. Overview of the research framework in Papers I-IV. TRL refers to technology readiness level; T_0 refers to present time; T_f refers to future time when each battery type reaches its highest TRL; rectangle boxes refer to the production processes of the battery; rectangle boxes with a dash line refer to production processes at T_0, while rectangle boxes with a solid boundary line refer to production processes at T_f. LIBs, SIBs, ASSBs, OB refer to lithium-ion batteries, sodium-ion batteries, all-solid-state batteries, and all-organic battery, respectively. Note: T_f represents the point at which each specific battery technology reaches its highest TRL, with the absolute timing varying across different technologies.

This thesis is based on the research presented in Papers I-IV (Figure 1). Papers I and II focus on assessing the environmental performance of an all-organic battery. Primary laboratory (lab) data for the synthesis of the all-organic battery were provided by the Nanotechnology and Functional Materials group at Uppsala University, which was used to construct the life cycle inventory (LCI). The synthesis processes involved many fine chemicals for which no existing LCI data was available. Consequently, substantial efforts were made to develop a comprehensive LCI for these chemicals. This was accomplished by identifying their production routes from literature and patents and tracing back their production chains until all input materials were included in the LCA database (ecoinvent). Missing data, such as cooling water, solvent consumption, solvent recycling, and energy consumption, were estimated using empirical factors and thermal equations. Building on the lab synthesis route that was identified in Paper I, Paper II scaled up the system to industrial production processes. Specifically, it recalculated the quantities of essential input materials, and the energy required for each unit process using the same empirical factors and thermal equations employed in Paper I. A prospective LCA (Paper II) was then conducted at T_f, based on the scaled-up system, which also considered future battery performance (Figure 1). For ASSBs (Papers IV) and SIBs (Paper III), which have relatively high Technology Readiness Levels (TRL) for both the battery technology and battery components materials, more data was available to support the creation of future scenarios. Consequently, these two LCA studies considered a longer time perspective (T_f and forward, Figure 1). The release of the Python tool Premise (Sacchi et al., 2023), which combines the outcomes of integrated assessment models with the ecoinvent LCA database, facilitated the consideration of background system changes for this analysis. Additionally, an increasing understanding of battery design and working principles led to the development of two battery dimensioning models. These two models provided essential inputs regarding the quantities of materials and energy required for battery production and corresponding battery performance, which ensured a fair comparison between different battery technologies with the same shape and dimensions.

3. Background

3.1 Current battery technologies

The use of batteries dates back to over a century, beginning with lead-acid batteries (LABs), which were introduced in 1859 by French physicist Gaston Planté (Vangapally et al., 2023). These batteries, which represent the oldest form of rechargeable batteries (Vangapally et al., 2023), are renowned for being the most economical secondary power source. Their high recycling rate of over 99%, exceptional cold-cranking capabilities, and robust cycle life stability have rendered them as the preferred choice for energy storage across various sectors (Vangapally et al., 2023). These attributes have enabled them to dominate the market for more than a century. In 2021, the LAB market was valued at US $43 billion (Statista, 2022). Their applications are diverse, ranging from automotive starting-light-ignition to uninterruptible power supplies (UPS) for homes and solar street lighting (Vangapally et al., 2023). Innovations in the recent two decades have increased LABs lifespan by 30-35%, signifying ongoing advancements in this technological field (Zhao et al., 2021). Nonetheless, their relatively low energy density, both gravimetric (Wh/kg) and volumetric (Wh/L), continues to pose challenges. Following LABs, nickel-cadmium (NiCd) batteries, which were discovered by Ernst Waldemar Jungner in 1899, have been extensively used in rechargeable applications for over a century, particularly in portable devices such as video cameras and power tools, due to their effective voltage maintenance and charge retention (Wang et al., 2022). However, the toxicity of cadmium (Cd) has led to regulatory restrictions on NiCd use in many countries, diminishing their presence in the 3C electronics markets (3C: computer, communication, and consumer electronics) (Wang et al., 2022). As an environmentally friendly alternative, nickel-metal hydride (NiMH) batteries emerged in 1967 and were widely adopted in vehicles by the mid-1990s. NiMH batteries require less maintenance and offer a 40% higher energy density compared to Ni-Cd batteries (Zhao et al., 2021).

Currently, lithium-ion batteries (LIBs) are the dominant technology in both EV and storage applications (International Energy Agency, 2024a). Commercialized in the 1990s, LIBs quickly became the most popular and rapidly expanding technology within the battery market. LIBs offer superior gravimetric (Wh/kg) and volumetric (Wh/L) energy densities, extended cycle life, long shelf life, minimal maintenance requirements, fast charging capabilities, and a wide operational temperature range (International Energy Agency, 2024a). These characteristics have established LIBs as a critical component in various applications. Lithium cobalt oxide ($LiCoO_2$, LCO), the first cathode material used in rechargeable LIBs, was introduced by Goodenough in 1980 (Mizushima et al., 1980) and has since become a dominant battery chemistry in portable 3C devices (Bauer et al., 2022; Wang et al., 2020). Current research aims to further enhance LCO's performance for thin, lightweight, and flexible electronic products (Wang et al., 2020). However, due to the high cost of cobalt and the relatively low energy density, LCO is considered unsuitable for powering large devices, such as stationary energy storage and electric vehicles (EVs), which require numerous battery cells (Wang et al., 2020). The automotive industry has been exploring cathode materials that offer higher energy capacity, reduced raw material costs, improved cycle life, and enhanced safety (Frith et al., 2023). This has encouraged intensive research into cobalt-reduced or even cobalt-free cathode chemistries, including lithium nickel manganese cobalt oxide (NMC), lithium nickel cobalt aluminium oxide (NCA), and lithium iron phosphate (LFP) for EVs (Bauer et al., 2022). Substituting cobalt with nickel can increase cathode and battery cell capacity while also reducing costs by over 50% (Frith et al., 2023; Passerini et al., 2024). Recent advancements have enabled battery cells with high-nickel NMC811 cathodes to achieve a specific energy of over 270 Wh/kg (Frith et al., 2023). The automotive industry is also working to increase the energy density of EV batteries by adopting cell-to-pack configuration (Frith et al., 2023). It was reported that this approach can improve the volumetric and gravimetric energy densities of LFP battery packs from 210 Wh/L to 330 Wh/L and from 135 Wh/kg to

160 Wh/kg, respectively (X. G. Yang et al., 2021). Regarding anode active material, commonly used materials include graphite, lithium-titanate ($Li_4Ti_5O_{12}$, LTO), and silicon/carbon composites.

3.2 Social, environmental, and technical challenges of current Li-ion batteries and the need for alternatives

The predominant battery technologies, LIBs, face several significant challenges. Firstly, they rely on critical minerals such as lithium, cobalt, nickel, and graphite, which has raised concerns over child labour, geopolitical tensions, and supply risks. Secondly, the technical and economic performance of LIBs cannot fully address the needs of all market segments. These issues are discussed in this section.

3.2.1 Issues related to cobalt mining

Cobalt (Co) mining has substantial environmental and social impacts. Environmental impacts include air and water pollution from dust and chemical runoff, which negatively affects both the mining sites and surrounding communities (Sovacool, 2019). This pollution contributes to habitat destruction, loss of biodiversity, soil erosion, and land degradation (Sovacool, 2019). Additionally, the global Co supply chain is characterized by geopolitical complexities, due to a significant portion of the world's reserves being located in geopolitically sensitive areas. At present, the Democratic Republic of the Congo (DRC) supplies approximately 70% of the global cobalt and holds 48% of the reserves (USGS, 2022). However, Co mining in the DRC is associated with serious issues, such as exploitation, child labour, and dangerous working conditions, which are driven by the intense economic pressures (Sovacool, 2019).

Artisanal mining, which is prevalent in the DRC, often involves unsafe working conditions due to the lack of appropriate and necessary safety equipment (Sovacool, 2019). The miners, particularly those involved in small-scale artisanal operations, face risks from mine collapses and exposure to toxic substances (Sovacool, 2019). This not only endangers the miners' health but also poses health risks to the local communities. A case study in Kolwezi, DRC, found that residents living near artisanal cobalt mines had significantly higher levels of Co in their urine and blood compared to those in less affected areas. Children, in particular, exhibited severe health effects, including oxidative DNA damage (Nkulu et al., 2018).

Furthermore, cobalt mining is associated with various social issues including community displacement, infringement on the rights of indigenous peoples, and challenges related to corruption and governance (Sovacool, 2019). Despite these problems, many communities in the DRC depend heavily on mining for their livelihoods due to the scarcity of alternative employment opportunities. Although mining revenue contributes to public infrastructure, education, and health services, these benefits are often limited and unevenly distributed (Sovacool, 2019). What's more, in some regions, mining is not only an economic pursuit but also an important part of the local cultural identity, fostering a sense of pride and belonging among community members. All these factors together increase the complexity of addressing the problems associated with Co mining

3.2.2 Issues related to lithium mining

Lithium (Li) is primarily extracted from two sources: brine and spodumene pegmatite ("hard-rock"). Brine extraction requires pumping saline groundwater to the surface and evaporating it in large ponds, a process that consumes between 100 to 800 m³ of water per tonne of lithium carbonate produced (Vera et al., 2023). This significant water usage places a strain on water resources, especially in arid regions. Further, more than 90% of the salts, aside from lithium chloride, crystallize as waste in these ponds (Vera et al., 2023), which has severe environmental impacts on local ecosystems. The environmental impacts of Li mining have also led to conflicts amongst local communities and indigenous people. Water shortages and ecosystem disturbances affect the local agriculture and livestock, which threatens both livelihoods and cultural heritage (Owen et al., 2023). Moreover, Li mines are often located near land that is inhabited by indigenous and local communities. These groups are frequently excluded from the decision-making processes regarding mining projects on their land, leading to violations of their rights to consultation and free, prior, and informed consent (Owen et al., 2023).

Furthermore, the long period that is required to develop a mine into operation can lead to imbalances between supply and demand, therefore driving up material costs (Manalo, 2024). For example, in May 2022, an insufficient investment in expanding supply capacity caused a significant increase in Li prices, rising over seven times of their early 2021 levels (International Energy Agency, 2024b). According to the International Energy Agency's (IEA) Announced Pledges Scenario (APS), Li demand could reach 500 kilotonnes by 2030. This demand will require the establishment of approximately 50 new average-sized mines. The APS also cautious that the Li supply may be insufficient in supporting the energy transition, highlighting the need to address these systemic challenges (International Energy Agency, 2024b). Furthermore, the uneven global distribution of Li resources has exacerbated these challenges (Greim et al., 2020). Indeed, more than 50% of Li are currently mined in Australia (International Energy Agency, 2024b). Around 70% of Li resources are concentrated in the "Lithium Triangle" region of Bolivia, Chile, and Argentina, where resource management is often inefficient (Eftekhari, 2019; Halkes et al., 2024). This geographic concentration, combined with the potential future imbalance between supply and demand, is likely to amplify supply chain pressures.

3.2.3 General supply chain risks and technical challenges

The significant geographical concentration of key battery minerals and materials introduces various vulnerabilities to the supply chain. China plays an important role in the LIB production chain, from mineral mining, material processing and refining, battery component producing, to battery manufacturing. Based on International Energy Agency (2024b), China accounts for 75% of global LIB production, 70% of cathodes production and 85% of anodes production. This geographical concentration extends to the processing and refining of key LIB minerals, with more than half of the world's Li, Co, and graphite being processed in China. Further, China is a major player in graphite mining, with it being responsible for 80% of global production (International Energy Agency, 2024b). The concentration of these critical activities in China, along with the fact that Australia mines over half of the world's lithium and the DRC mines 70% of global Co, highlights the vulnerabilities and supply chain risks associated with LIB production. The resilience of battery supply chains was tested during the COVID-19 pandemic and the war in Ukraine, which exposed concerns over nickel supply disruptions. The increase in nickel prices in 2022 reflected these concerns, as Russia is the largest producer of battery-grade nickel (International Energy Agency, 2024b). However, innovation in new chemistries, such as sodium-ion batteries, can help alleviate some of the current pressure on the supply chain for these minerals (International Energy Agency, 2024b).

Additionally, concerns on the safety issue and the vehicle driving range are significant barriers to EV adoption (Noel et al., 2019; Pevec et al., 2020). The International Energy Agency (2024b) indicates that customers have a preference for larger and longer driving range vehicles such as sports utility vehicles (SUVs), which comprise of more than half of the electric models available globally. This suggests that there is a need for batteries with a higher specific energy, such as all-solid-state batteries, which could enable longer driving ranges on a single charge.

3.3 Emerging batteries

Looking ahead, advancements in battery technology are predominantly focused on overcoming the limitations of current systems to meet the increasing demand. The requirements for battery technologies vary across different application areas. For instance, in the field of portable electronics, there is a growing trend towards flexible and bendable devices, which require batteries that accommodate such innovative designs (Shan Zhang et al., 2022). Additionally, in developing regions and certain applications where cost is a critical factor, customers prioritize cost-effective solutions (IEA, 2024). Meanwhile, in the EV sector, there is a strong demand for batteries that offer both high energy density and enhanced safety (IEA, 2024). It is important to note that no single type of battery can address all of the present challenges and requirements across different applications. As a result, there will be diverse batteries within the battery market to meet varying customer demands. The diversity in battery chemistries can lead to a more varied supply chain of materials, which can help to reduce supply chain risks. This section introduces three types of emerging batteries that seem promising for use in different applications.

3.3.1 All-organic batteries

Organic batteries, which use organic materials as electrode active materials, are emerging as promising power sources for flexible portable devices in various applications. These range from healthcare (e.g., wearable devices), logistics (e.g., intelligent packaging), displays, and soft robotics

(Chung and Kang, 2009; Cima, 2014; Schaefer and Cheung, 2018; Son et al., 2014). These organic materials can theoretically be derived from biomass and therefore offer a sustainable resource alternative. Researchers believe that organic electrode materials will excel in the "post Li-ion battery" era, characterized by their sustainability, flexibility, tunability, and cost effectiveness (Song and Zhou, 2013). This technology not only introduces novel life experiences but also supports the transition toward a hyper-connected society (Choi, 2014). Furthermore, the absence of metals in these batteries simplifies end-of-life treatment, which allows for recycling or incineration using the same waste treatment route as the product they power. Despite the growing interest in organic batteries, their development is still in early stages, and a consensus on the optimal design of organic battery material has not yet been reached. The variability of organic materials provides extensive opportunities for tailoring material properties (Muench et al., 2016). Polymer-based electrode materials have shown highly promising features, suggesting a move towards adopting polymer-active materials as a general design principle (Hager et al., 2020). A key advantage of polymeric materials is their inherent stability. They resist decomposition and dissolution when in contact with electrolytes (Muench et al., 2016). Also, the processability and formability inherent in polymeric materials enhances their attractiveness (Muench et al., 2016). It should be noted that although these organic materials can theoretically be derived from biomass, they are currently produced using fossil fuels (Emanuelsson et al., 2017). Further research is needed to transition to biomass-based precursors and fully uncover their benefits.

Among the various polymer materials, PEDOT (poly(3,4-ethylenedioxythiophene)) stands out because of its high electrical conductivity and excellent stability under ambient conditions (Hager et al., 2020). The recent advancements in material science have significantly increased PEDOT's conductivity, with it now approaching that of highly conductive metals such as silver and copper, by only an order of magnitude lower (Gueye et al., 2020; Kim et al., 2017). This high conductivity is essential for applications that require efficient charge transport. Additionally, the stability of PEDOT in its doped state surpasses that of other conducting polymers, which is a crucial benefit that remains even in the presence of atmospheric oxygen and moisture (Gueye et al., 2020; Kim et al., 2017). This stability addresses performance degradation issues that are commonly faced by other organic conductive materials and is vital for the long-term reliability and functionality of devices that incorporate PEDOT (Gueye et al., 2020). Furthermore, PEDOT’s intrinsic properties (including its electrochemical activity and compatibility with various doping methods and processing techniques), allow for the customization of its electrical, optical, and mechanical properties to meet specific requirements (Gueye et al., 2020). This adaptability supports PEDOT’s integration into a broad array of technology platforms, including flexible and wearable electronics, where conventional materials may not be ideal due to cost, rigidity, or processing constraints (Gueye et al., 2020).

3.3.2 All-solid-state batteries

All-solid-state batteries (ASSBs), which employ solid electrolytes instead of liquid, enable the use of lithium metal as an anode, thus significantly enhancing the battery energy density and allowing for bipolar electrode configurations to maximize spatial efficiency (Sun, 2020). The "Solid-State Battery Roadmap 2035+" by Schmaltz et al. (2022) estimates that emerging SSBs could reach gravimetric energy densities of 350 to 500 Wh/kg, depending on the electrolyte material used. Their high energy density has attracted interest from major automotive companies such as Toyota, BMW, Dyson, and Honda (Quartarone and Mustarelli, 2011; Yang et al., 2021a).

The use of solid electrolytes in ASSBs eliminate the risks of leakage and flammability inherent in LIBs. This significantly reduces the combustion risks and addresses major safety concerns, such as explosions or fires in the event of a breach (Sun, 2020). Moreover, ASSBs can also operate over a broader temperature range (−30 to 100 °C), therefore improving its performance under extreme weather conditions and expanding the viability of EVs (Kim et al., 2015). Despite these benefits, ASSBs face challenges which include difficulties in achieving high ionic conductivity comparable to that of liquid electrolytes, overcoming low Coulombic efficiency and power performance issues due to interfacial resistance, and enhancing the electrochemical stability of the solid electrolytes. Additionally, sensitivity to ambient atmosphere requires a careful handling of SEs under inert conditions (Muramatsu et al., 2011). Ongoing research into both organic and inorganic materials for SEs shows the potential to overcome these hurdles (Albertus et al., 2021; Sun, 2020).

Solid-state electrolyte materials can be classified into two main categories: ceramic-based and polymer-based categories. Ceramic-based electrolytes, further divided into oxide-based, sulfide-based, and halide-based, offer high ionic conductivity and thermal stability (Yang et al., 2021a). For example, oxide-based electrolytes like perovskite ($Li_3xLa_{2/3}{-}xTiO_3$, LLTO), NASICON-type structures ($Li_{1.3}Al_{0.3}Ti_{1.7}(PO_4)_3$, LATP; $Li_{1.5}Al_{0.5}Ge_{1.5}(PO_4)_3$, LAGP), and garnet-type structures ($Li_7La_3Zr_2O_{12}$, LLZO) are known for their superior oxidation and thermal stabilities (Yang et al., 2021a). However, sulfide-based electrolytes, such as $Li_{10}GePS_{12}$ and Li_6PS_5Cl, although having higher ionic conductivity than oxides, struggle with chemical instability and manufacturing challenges (Schnell et al., 2019; Zhao et al., 2020). Compared to ceramic electrolyte, polymer electrolytes offers greater flexibility, improved electrode-electrolyte intimacy, and simpler processing. These electrolytes can be further improved by adding ceramic particles to reduce crystallization and enhance ionic conductivity, thus offering a blend of flexibility and effective battery performance (Huang et al., 2021; Zhao et al., 2019).

3.3.3 Sodium-ion batteries

Sodium-ion batteries (SIBs) operate on the same fundamental principle as LIBs, relying on the intercalation of alkali ions into electrodes during charge and discharge cycles (Tapia-Ruiz et al., 2021). This operational similarity suggests that existing LIB manufacturing infrastructure could be adapted for SIB production without significant additional investment (Tapia-Ruiz et al., 2021). The rapid development of SIBs, especially in areas such as electrode densities and coulombic efficiencies, benefits from the foundational research and experience gained in LIB technology (Rudola et al., 2021; Tapia-Ruiz et al., 2021).

Unlike LIBs, SIBs use sodium, which is abundant and widely available, compared to the relatively scarce and unevenly distributed lithium (Usiskin et al., 2021). This shift could mitigate some of the supply constraints and geopolitical risks that are currently associated with lithium mining. For anodes, SIBs cannot use commercially available graphite due to issues with sodium-carbon intercalation. Instead, hard carbon is employed, even though it reacts less with sodium than lithium does in graphite, on a per unit mass and volume basis (Tapia-Ruiz et al., 2021). Additionally, SIB chemistry allows the use of aluminium (Al) for both anode and cathode current collectors, unlike LIBs, which require copper (Cu) for the anode due to lithium’s reactivity with Al (Zhang et al., 2021). This switch not only significantly lowers cell costs and battery weight but also mitigates the risk of over-discharge in organic solutions. Moreover, substituting Cu with Al could reduce both the cost and battery mass. However, this swift may cause increase in volume (Vaalma et al., 2018).

Performance-wise, SIBs exhibit a lower redox potential (−2.71 V for sodium vs. −3.04 V for lithium), greater atomic mass (23 g/mol for sodium, 7 g/mol for lithium), and larger ionic size (1.02 Å for sodium, 0.76 Å for lithium) than lithium, which collectively lower the theoretical energy density of SIBs (Tapia-Ruiz et al., 2021; Vaalma et al., 2018). However, SIBs are considered to be safer and more suitable for rapid charging across a broader temperature range (−20 to +60 °C) compared to LIBs (Liu et al., 2020).

Several companies are at the forefront of commercializing SIBs. Faradion Limited, a leader in the SIB field, focuses on high energy density cathodes (layered oxide) paired with hard carbon anodes. Their product cells currently show energy and power densities between LCO battery and LFP battery, with aims to enhance SIB performance to specific energy levels of 210 Wh/kg, specific power of 2000 W/kg, and a cycle life of 8000 cycles at 80% depth of discharge (Rudola et al., 2021; Tapia-Ruiz et al., 2021). The company Tiamat specializes in polyanionic materials, targeting the fast-charging capabilities of their batteries, which offer specific energy of 100–120 Wh/kg and excel in durability, sustaining over 4000 cycles with more than 80% capacity at a 10C rate. This positions Tiamat's technology as a versatile option for applications such as e-bikes, e-scooters, and automotive systems (Broux et al., 2019). Companies such as Novasis Energies, Altris AB, and Natron Energy are exploring Prussian blue analogue batteries that avoid using critical metals and are noted for their exceptional cycle life. Hi Na Battery Technology Co., Ltd. focuses on Na-Fe-Mn-Cu oxide cathodes and anthracite carbon anodes, producing batteries optimized for a variety of applications, from e-bikes to household energy storage systems. Recently, car manufacturers have started implementing SIBs in vehicles with ranges of up to 400 km (Batteries News, 2022). Such developments underscore the growing consensus on the potential of SIBs in the battery market.

3.4 Life cycle assessment methodologies of emerging batteries

It is essential to conduct an environmental assessment during the battery technologies' early development stage to gain a better understanding of their environmental performance and to avoid the unintended environmental consequences. LCA is a widely used tool for quantifying environmental impacts and identifying environmental hotspots over the life cycle of products, processes and services (Hauschild et al., 2018), and is commonly applied in studies on batteries (Porzio and Scown, 2021). The LCA framework consists of four phases: goal and scope definition, life cycle inventory analysis (LCI), life cycle impact assessment (LCIA), and interpretation (ISO, 2006a, 2006b).

In the goal and scope definition phase, the goal of the study, target audience, the production system boundary, geographical and temporal boundaries, and the functional unit(s) are established. After defining the goal and scope, the LCI phase involves collecting all input and output flows of the studied system. Input flows include resources directly extracted from the environment (known as elementary flows), materials produced by human activities or the technosphere (referred to as intermediate flows), and energy inputs. Output flows consist of the product(s), emissions released into the environment (classified as elementary flows), and waste that requires further processing within the technosphere (classified as intermediate flows). In this phase, all inventory data are scaled to align with the functional unit. Next, the LCIA phase translates these scaled elementary flows into environmental impacts using the selected LCIA method(s). This process involves selecting impact categories, classification and characterization. During classification, each elementary flow i is assigned to the environmental impact categories it contributes to. Characterization involves calculating the impact scores (IS_c) for each impact category c by weighting all elementary flows E_i based on their relative contribution (referred to as characterization factors CF_i) to the environmental issue c, and summing them up (Equation 3.1).

$$IS_c = \sum_i (CF_i \times E_i) \tag{3.1}$$

When conducting a LCA on emerging batteries, it is essential to identify the maturity level of the batteries during the goal and scope definition to ensure clear communication. The Technology Readiness Level (TRL) is a widely adopted metric used to assess the maturity of technologies, ranging from TRL 1 (the lowest level, where basic principles are observed) to 9 (the highest level, where the actual system is proven in an operational environment) (Table 1). In this thesis, the TRL framework defined by the European Commission is employed to quantify the maturity of emerging battery technologies that are studied (European Commission, 2014).

Table 1. Technology readiness level and its description (European Commission, 2014).

TRL	Description
1	Basic principles observed
2	Technology concept formulated
3	Experimental proof of concept
4	Technology validated in lab
5	Technology validated in relevant environment (industrially relevant environment in the case of key enabling technologies)
6	Technology demonstrated in relevant environment (industrially relevant environment in the case of key enabling technologies)
7	System prototype demonstration in operational environment
8	System complete and qualified
9	Actual system proven in operational environment (competitive manufacturing in the case of key enabling technologies; or in space)

The function of a battery cell is to store and deliver energy, so the functional unit should be align with this purpose (Porzio and Scown, 2021). Ideally, if sufficient data are available to conduct a LCA across the entire life cycle of the battery cell, a cradle-to-grave impact assessment should be performed based on a functional unit of 1 kWh of energy stored or delivered over the battery's lifetime, as shown in Equation 3.2.

$$IS_c = \frac{IS_{c,battery\ cell} + IS_{c,\text{use phase}} + IS_{c,\text{EoL}}}{lifetime\ energy\ stored} \tag{3.2}$$

$IS_{c,battery\ cell}$ represents the environmental impact associated with producing one battery cell for the impact category c. Similarly, $IS_{c,\text{use phase}}$ and $IS_{c,\text{EoL}}$ refer to the environmental impact caused by the use phase and end-of-life (EoL) of one battery cell, respectively. For emerging batteries, data on the use phase and EoL are often incomplete or unavailable.

The impact score for the battery cell, $IS_{c,battery\ cell}$, can be calculated by multiplying the impact score per unit of input flows, $IS_{c,i,unit}$, by the amount of that input flow a_i, as shown in Equation 3.3. Input flows include the energy required for battery manufacturing (a_i in kWh) and battery components (a_i in kg) such as the anode, cathode, electrolyte, current collector, separator, and battery casing.

$$IS_{c,battery\ cell} = \sum_i IS_{c,i,unit} \times a_i \qquad (3.3)$$

The energy stored over a battery's lifetime (in kWh) can be calculated by considering several key factors (Equation 3.4): the battery capacity (in Wh), the number of cycles a battery cell can perform before reaching its EoL, the portion of the battery's theoretical capacity that can be safely used without damaging the battery (known as the state-of-charge, or SoC), the percentage of usable capacity discharged in each cycle (known as depth of discharge, or DoD), and the ratio of useful energy output to the energy input (referred to as energy efficiency, EE) (Peters et al., 2021).

$$lifetime\ energy\ stored = \\ battery\ capacity \times cycle\ life \times \mathrm{SoC} \times DoD \times EE \times 10^{-3} \qquad (3.4)$$

The battery's theoretical capacity (in Wh) can be estimated using the specific capacity of the cathode active material ($capacity_{cam}$ in Ah/kg), the mass of the cathode active material (m_{cam} in kg), and the average discharge voltage (Zhang et al., 2024), as shown in Equation 3.5.

$$battery\ capacity = m_{cam} \times capacity_{cam} \times \mathrm{voltage} \qquad (3.5)$$

Equation 3.2-3.5 indicate three types of data required for conducting an LCA of emerging batteries: data related to the battery technology, data related to the foreground system (such as $IS_{c,i,unit}$ in Equation 3.3), and data related to the background system (used directly and indirectly in calculating $IS_{c,i,unit}$). Battery technology data include battery composition (a_i in Equation 3.3 and m_{cam} in Equation 3.5) and battery performance (Equation

3.4, and 3.5). The foreground system refers to the parts of the system in which stakeholders have direct control or significant influence, while the background system includes the parts of the system not directly controlled by the decision-maker or central to the study (Hauschild et al., 2018).

LCA can be conducted from two temporal perspectives when assessing emerging battery technologies (Figure 2). The first approach is to perform the assessment at the current time (T_0), using small-scale foreground data (at lab- or pilot-scale), current LCA background databases (such as ecoinvent), and small-scale battery composition and performance data. This is typically referred to a lab-scale LCA or a pilot-scale LCA (Moni et al., 2020), providing insights into the immediate environmental performance based on current technological capabilities. The second approach is to explore the system in the future (T_f), when the batteries are developed and produced at large scale (i.e. at their highest TRL). This prospective approach, known as prospective LCA (Arvidsson et al., 2024), considers potential changes in production processes (both for the foreground and the background system) and improvements in battery design and performance.

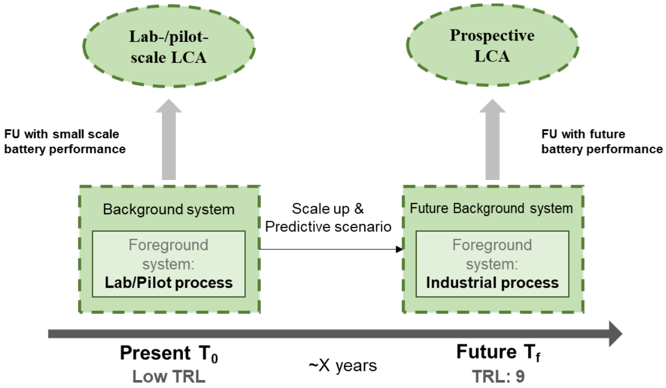

Figure 2. Life cycle assessment of emerging technologies.

To upscale small-scale chemical processes in the foreground system, simulation software such as Aspen can be employed. Additionally, other methods such as process engineering equations, learning curves, empirical parameters, cost curves, regression analysis, and power laws can also be used to provide estimates (Bergesen and Suh, 2016; Caduff et al., 2014; Capello et al., 2005; Geisler et al., 2004; Piccinno et al., 2016). Regarding future background system modeling, some studies assume an unchanged background system due to short-term scenarios (Arvidsson et al., 2014; S. Zhang et al., 2022), while others account for changes by integrating the outcomes from integrated assessment models (IAMs) to update the corresponding production processes and emissions in the LCA database (Xu et al., 2022; Zhang et al., 2024). It is important to note that although discussions have stressed the importance of considering background system changes (Arvidsson et al., 2014; Arvidsson et al., 2018), this practice was not common until recently due to the complexity of modifying background databases. The recent development of the Python tool Premise has simplified this process, making it more feasible to account for such changes (Sacchi et al., 2022).

There is no consensus on a standardized methodology for assessing the environmental performance of emerging battery technologies, as each approach has its own limitations and advantages (Passerini et al., 2024). Lab- or pilot scale LCA may provide relatively accurate environmental impact assessment for early-stage technologies, but as production scales up, both the overall environmental impact scores and hotspots can change significantly due to improvements in material and energy efficiency, changes in the background system, and advances in battery technology. Previous LCA studies have shown that environmental impact scores can vary by several orders of magnitude between lab-scale and industrial-scale LCAs (Troy et al., 2016; Villares et al., 2017). This creates challenges when relying on lab-scale LCA results for long-term decision-making (Pallas et al., 2020a).

3.5 Review of LCA studies on emerging batteries

To the best of my knowledge, Paper I and II are the only LCA studies conducted on all-organic batteries (Shan Zhang et al., 2022; S. Zhang et al., 2022). For ASSBs, Lastoskie and Dai (2015) assessed the environmental impacts of SSB cells and laminated cells for the EV application. Their analysis across various cell chemistries showed that SSBs generally exhibited lower environmental impacts, particularly those using lithium vanadium oxide (LVO) electrolytes. This can be attributed to the high specific energy of LVO, which offered advantages (reduced energy consumption) during the EVs use phase. Troy et al. (2016) conducted an early LCA of SSBs with lithium-lanthanum-zirconium-oxide (LLZO) electrolyte across lab, pilot, and industrial scales. Because of the early development stage of the SSB, the study did not include comparisons with existing battery technologies. Their results highlighted the substantial impact of electricity consumption during cell manufacturing. The results also revealed the sizeable reduction in environmental impacts while upscaling the process. Vandepaer et al. (2017) conducted an LCA on a SSB featuring an LFP cathode, a lithium metal anode and a polymer electrolyte. The study found that, compared to LIBs, the SSB performed better in terms of climate impacts and ozone depletion, but exhibited inferior performance in eutrophication. Keshavarzmohammadian et al. (2018) explored the environmental impacts of a SSB pack with a pyrite cathode for EV applications, finding that the climate impact was comparable to that of traditional LIBs, but energy demand were higher compared to that of traditional LIBs. They also expect the energy demand to be reduced with the increasing of production size. The primary contributors to environmental impacts were energy use in cell manufacturing processes, especially in dry rooms and during cathode paste production. J. Y. Zhang et al. (2022) conducted a lab-scale LCA on a SSB coin cell with a lithium-aluminium-titanium-phosphate (LATP) electrolyte. The study noted that the solid-state LATP cell required higher primary energy (2.6 MJ vs. 1.1 MJ) and produced roughly double the GHG emissions (0.1 kg CO_2-eq vs. 0.05 kg CO_2-eq) compared to a conventional LIB cell, primarily due to the energy-intensive production of the solid electrolyte. The study highlighted that reducing the electrolyte layer's thickness significantly lowered these environmental impacts, indicating the potential for manufacturing advancements to mitigate the technology's environmental footprint.

As for sodium-ion batteries, Peters et al. (2016) conducted a pioneering LCA to evaluate the cradle-to-gate environmental impacts of a layered-oxide SIB pack, and compared it to various LIB packs across six environmental impact categories. The results showed that SIBs had lower impacts on freshwater eutrophication and human toxicity than LIBs, with comparable impacts on global warming, fossil depletion, and terrestrial acidification. However, SIBs had higher impacts on marine eutrophication. The study also highlighted that battery cycle life is a key determinant of environmental performance. Peters et al. (2021) conducted a cradle-to-grave LCA on five different types of SIBs and compared them to LIBs. They developed a battery-dimensioning tool to estimate the required battery materials and corresponding battery performance. The results highlighted the importance of recirculate battery materials to reduce environmental impacts. Schneider et al. (2019) performed an LCA on a layered oxide SIB based on electrochemical modelling and found that SIB cannot outperform LIBs in terms of climate impact. Jasper et al. (2022) conducted a comparative LCA on a SIB for home battery system. This system was compared against three LIB chemistries using a functional unit (FU) of 1 kWh of delivered electricity. The SIB, which used a sodium nickel magnesium manganese titanium oxide cathode and a hard carbon anode, exhibited higher impacts on global warming potential, resource depletion, and freshwater toxicity throughout its lifecycle compared to the LIB systems. This was primarily due to its lower energy density, which required more material per unit of electricity produced.

4. Materials and method

4.1 Battery technologies

This section discusses the battery chemistries studied in this thesis, covering both the emerging batteries and the conventional batteries that are used as benchmarks. It describes the characteristics of the emerging batteries, the materials used for each battery component, and the battery dimensions. Common battery shapes on the market include pouch, prismatic, and cylindrical cells, each with its own advantages and disadvantages, making them suitable for different applications.

4.1.1 All-organic battery and flexible Li-ion battery (Paper I and II)

The all-organic battery cell assessed in this study was developed by the Nanotechnology and Functional Materials group at Uppsala University (Strietzel et al., 2020). The battery cell is modelled as a single layer thin film cell, to maintain its bendable feature. At lab scale, the battery cell has a mass of 483.23 mg, with an active area of 9 cm^2 (3 cm × 3 cm), and a casing area of 12.25 cm^2. It features a specific capacity of 60 mAh/g based on the electrode active material, leading to an overall capacity of 1.08 mAh. It has an average discharge voltage of 0.4 V, and delivers a specific energy of 0.9 Wh/kg. Strietzel et al. (2020) reported that this battery maintains 85% of its initial capacity after enduring 500 charge-discharge cycles, can achieve a full charge in merely 100 seconds, and sustains its performance robustly at temperatures as low as −24 °C.

The battery cell is composed of six components: the cathode, anode, electrolyte, current collector, separator, and the cell casing. Electrode material uses pure conducting redox polymers (CRPs), without binders or conductive additives needed. These CRPs are characterized by their polymeric backbones with trimeric repeat units (EPE), and two distinct pendant groups: hydroquinone (QH_2) and naphthoquinone (NQ) for the cathode and anode, respectively. In the synthesis of EPE, two moieties of 3,4-ethylenedioxythiophene (EDOT, denoted as E) are attached to the alpha positions of a central 3,4-propylenedioxythiophene (ProDOT, denoted as P) unit (illustrated in Paper I, Fig. S2). This backbone structure is used to enhance electronic conductivity while simultaneously decreasing the solubility of the conducting redox polymers (CRPs) within the electrolyte. The pendant groups: benzoquinone/hydroquinone (Q/QH_2) for the cathode and naphthoquinone/naphthohydroquinone (NQ/NQH_2) for the anode, act as the capacity carriers engaging in the quinone/hydroquinone redox reaction, which involves a two electron/two proton ($2e^-/2H^+$) transfer during the charge and discharge cycles of the organic battery. QH_2 and NQ moieties are attached to the trimeric EPE structure's central unity to synthesize the monomers $EP(QH_2)E$ and EP(NQ)E (depicted in Paper I, Fig. S2). Following this, the monomers are polymerized to yield the CRPs: $pEP(QH_2)E$ and pEP(NQ)E, which are used as the active materials for the cathode and anode, respectively.

To enable a better understanding of the environmental performance of the all-organic battery, a flexible and bendable LIB was included as reference (Paper II) (Hu et al., 2010). For the composition of the flexible LIB, LTO and LCO were used as anode and cathode active materials, respectively. A sheet of commercial paper was used as the separator and a highly conductive carbon nanotube film as the current collector for the both electrode. The battery cell was assumed to be sealed with polydimethylsiloxane. The electrolyte is $LiPF_6$ in EC and DEC. Information on battery composition and performance is included in Paper II. It should be noted that materials used in the LIB are extensively commercialized. The optimized commercial production route offers a distinct advantage regarding material and energy use efficiency over the organic batteries (Mackanic et al., 2020; Wehner et al., 2021).

4.1.2 All-solid-state batteries (Paper IV)

Two ASSBs were considered. The first one used LFP as the cathode, pure lithium as the anode, and poly(ethylene oxide) (PEO)- lithium bis(trifluoromethanesulfonyl)imide (LiTFSI) as the solid-state electrolyte. The second ASSB featured NMC811 as the cathode, pure lithium as the anode, and lithium lanthanum zirconium oxide ($Li_7La_3Zr_2O_{12}$, LLZO) as the solid-state electrolyte. Two conventional LIBs, one with LFP and the other with NMC811 as the cathode, both using a $LiPF_6$-based liquid electrolyte, were included as benchmarks.

To ensure a fair comparison, all battery cells were standardized to a pouch format with dimensions of 67 mm in width, 112 mm in length, and 20 mm in height (Kevin W et al., 2022; Lee et al., 2020). The pouch cell format was selected because it is considered the most suitable shape for SSBs. The cells were manufactured by stacking multiple layers of repeating units, sealed within an Al polymer bag. For the ASSBs, a bipolar cell design was used, where each repeating unit consisted of an Al current collector, a cathode, a solid-state electrolyte, and an anode. For LIBs, each repeating unit consisted of an Al current collector foil with double-side coated cathode, a separator, and a copper current collector foil with double-side coated anode. A battery-dimensioning model was developed to calculate the material composition for each battery material and its specific energy. Details of the battery dimensioning model and the composition results can be found in Paper IV.

4.1.3 Sodium-ion batteries (Paper III)

Three SIBs were considered. Three cathode materials were selected based on their market potential: layered oxide $Na_{1.1}(Ni_{0.3}Mn_{0.5}Mg_{0.05}Ti_{0.05})O_2$ (NMMT), polyanion $Na_3V_2(PO_4)_2F_3$ (NVPF), and prussian blue analogues $Na_2FeFe(CN)_6$ (NaPBA) (Rudola et al., 2021; Tapia-Ruiz et al., 2021; Usiskin et al., 2021). The remaining components of all three SIBs were identical: hard carbon was used as the anode, Al foil served as the current collector for both electrodes, and $NaPF_6$ were used as the electrolyte. For comparison, conventional LIBs with LFP and NMC811 cathode materials were included as benchmarks.

To ensure a fair comparison, all battery cells were standardized to the 21700 cylindrical format, measuring 21 mm in diameter and 70 mm in height. A battery-dimensioning model was developed to calculate the material composition and specific energy for each battery chemistry. This model assumed a uniform thickness for the battery roll, comprising of layers of an Al current collector foil with double-side coated cathode, a separator, and an Al current collector foil with double-side coated anode, all wound in an Archimedean spiral. The Archimedean spiral function was used to determine the amount of material required for each component, considering layer thickness or electrode mass loading, material properties (such as density and porosity), and the battery cell's internal volume (Waldmann et al., 2020). The detailed battery-dimensioning model is presented in Paper III, SM 2, with the composition results summarized in Paper III, Table 1.

4.2 General methodology structure

The technological maturity of the studied battery technologies was assessed using the TRL as an indicator, as shown in Table 2.

Table 2. Technology readiness level of battery technologies, as well as their components at T_0.

	All-organic battery	All-solid-state batteries	Sodium-ion batteries
Battery technology	3-4	5 (Li-NMC811), 8 (Li-LFP)	8
Anode material	3-4	8	8-9
Cathode material	3-4	9	8-9
Electrolyte material	9	8-9	9
Other components	9	9	9

In this thesis, both a lab-scale LCA and a short-term prospective LCA (pLCA) were conducted for the all-organic battery (Papers I and II; Figure 3), while the long-term pLCA was applied to ASSBs (Paper IV, Figure 3), and SIBs (Paper III, Figure 3). The selection of these methodologies was guided by data availability or technology maturity of the batteries.

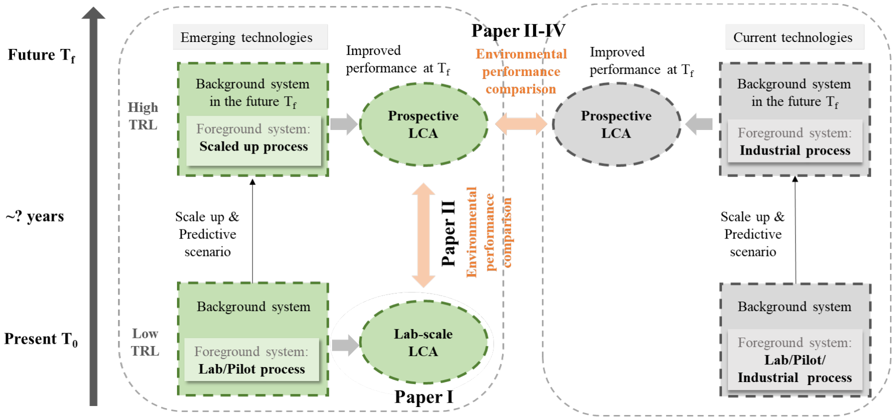

Figure 3. Overall methodology framework

For the all-organic battery, the TRL of both the battery technology and the electrode materials is currently around 3-4 (Table 2). The current lab-based synthesis route for the novel materials is complex and inefficient. Although it is expected that the synthesis route will be optimized at an industrial scale (by strategies such as shorting the synthesis route or changing synthesis methods and input materials), such improvements depend on future research and are difficult to predict at this stage (based on personal discussions with material chemists). Due to this the expected continuous chances in the production route, a long-term LCA is considered less meaningful. As a result, the focus for the all-organic battery is on identifying environmental hotspots in the production processes and supporting short-term decision-making for chemical engineers (focused on improving synthesis routes), process engineers (focused on upscaling), and battery researchers (focused on advancing battery technology).

For ASSBs and SIBs, the technologies are already relatively mature both at material and technology level. Literatures such as battery roadmaps and companies' development goals provide projections in the battery technology development, which can serve as a foundation for creating future scenario (Rudola et al., 2021; Schmaltz et al., 2022; Tapia-Ruiz et al., 2021). These data make long-term pLCA feasible for ASSBs and SIBs. The goal for studying both ASSBs and SIBs is to assess their future climate impact by 2025, 2030, 2040, and 2050. The LCA results offer more comprehensive insights for broader and longer-term considerations, which are not only relevant to engineers and researchers but also to policymakers involved in regulating these technologies.

The pLCA methodology used in this thesis integrates traditional LCA frameworks with scenario analysis, as illustrated in Figure 3 and 4. First, the timeline for these emerging technologies to reach market readiness was estimated based on their TRLs (Figure 3, from T_0 to T_f). Scenarios were then developed to explore the potential future state of the battery system at T_f (Figure 3 and 4), considering potential changes across three dimensions: the foreground system, the battery technology, and the background system (Figure 3 and 4). In the case of ASSBs and SIBs, the analysis extends beyond the time point T_f. Next, a pLCA study was conducted based on these projected future systems. The scenario development involved stakeholder (such as chemical engineers and battery researchers) engagement to ensure realistic assumptions for future conditions.

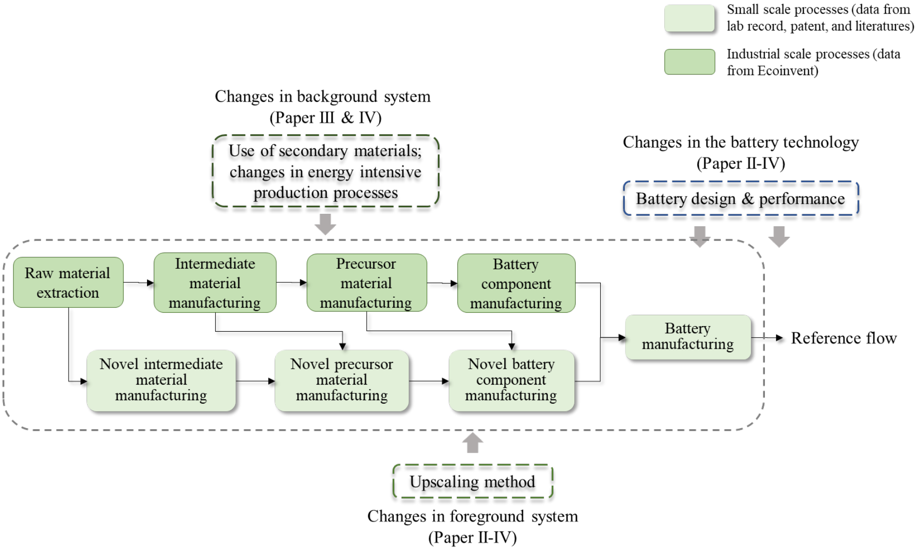

Figure 4. Methodology framework for conducting pLCA.

A FU of 1 kWh battery capacity and a cradle-to-gate system boundary were applied across all LCA studies. It needs to be noted that this FU is different from the one used in Paper II and III. The International Reference Life Cycle Data System (ILCD) 2011 midpoint method was used as the

LCIA method to evaluate the environmental impacts of the all-organic battery (Hauschild et al., 2011). Impact categories were identified following the guidelines from the Product Environmental Footprint Category Rules Guidance (PEFCR) (European Commission, 2018). For ASSBs and SIBs, only the climate impact is considered, and it was assessed using the IPCC Global Warming Potential (GWP) characterization factors over a 100-year time frame. The production of all studied batteries was assumed to take place in Europe. The impact scores for impact category c can be calculated as Equation 4.1.

$$IS_c = \frac{IS_{c,battery\ cell}}{battery\ cell\ capacity} \tag{4.1}$$

Where $IS_{c,battery\ cell}$ represents the impact score for producing one battery cell.

4.3 Scenarios generation and life cycle inventory

Based on the historical evolution of traditional LIBs, which reached industrial-scale maturity (TRL=9) from innovation stage within 12 years (Gross et al., 2018). It is assumed that with the accelerating pace of innovation and commercialization in the electronics sector (Gross et al., 2018), both the all-organic and the LIB technologies could achieve maximum TRL within a decade. In contrast, certain types of ASSBs are already in use in buses. Even though the studied ASSB chemistries in this study is still with relatively low TRL, given the rapid development and large investment in the field ASSBs, it is assumed that the studied specific battery chemistries could achieve the highest TRL by 2025. The same assumption applied also to SIBs, as they have reached the prototype stage with several companies announcing plans for mass production.

4.3.1 Future background system

For the all-organic battery study (Paper II), the background system is assumed to remain unchanged due to the short-term projection (Arvidsson et al., 2018; Villares et al., 2017). For SIBs and ASSBs studies, to simulate future background system transformations across various sectors and regions, the integrated assessment model REMIND was used. REMIND models potential changes in electricity sources, fuel generation technologies, production efficiencies in energy-intensive sectors, the deployment of Carbon Capture and Storage (CCS) technologies, and shifts in material and energy market shares under different scenarios (Baumstark et al., 2021). In the SIBs and ASSBs studies, these changes are considered under two scenarios: SSP2-NDC and SSP2-PkBudg500. The SSP2 scenario represents the Shared Socioeconomic Pathway 2, which assumes a continuation of current societal, economic, and technological trends (Riahi et al., 2017). The acronyms NDC and PkBudg500 denote two climate targets: the Nationally Determined Contributions and a pathway aligned with the 1.5°C temperature goal of the Paris Agreement, respectively. Following these two scenarios, that the global mean surface temperature rise could be limited to 2.5°C under SSP2-NDC and to 1.5°C under SSP2-PkBudg500 by 2100 relative to pre-industrial levels. These are referred to as the "2.5°C scenario" and the "1.5°C scenario" respectively in the following sections for simplicity. Following this, REMIND model outputs were used to update corresponding unit processes and emissions within the ecoinvent database (version 3.8 for SIBs, version 3.9 for ASSBs) using the Python package Premise (Sacchi et al., 2022).

ASSBs and SIBs studies also considers the use of recycled battery materials by incorporating recycled content in the input materials. This aligns with the EU's recent declaration on mandated levels of recycled content for critical battery materials such as Co, Ni, and Li (European Commission, 2023; Neef et al., 2021). In addition, recycled Al, Cu and manganese are considered, following scenarios from previous literatures (Born and Ciftci, 2024; European Aluminium, 2022; Joint Research Centre, 2024). These secondary materials are assumed to be sourced from used batteries and are reused in the upstream processes of battery production in the forms of lithium carbonate, cobalt sulfate, nickel sulfate, manganese sulfate, wrought Al alloy, and copper. Details can be read in Paper IV, supplementary material. It needs to be noted that the use of recycled minerals was considered in the SIBs study for this thesis but it was not included in Paper III.

4.3.2 Future foreground system and battery technology

The foreground system in this thesis includes the battery manufacturing processes and the production of novel battery components (Figure 4). For energy requirements in battery manufacturing, both the all-solid-state battery

(Paper II) and SIBs (Paper III) studies estimated their consumption using the LIB production process as a reference, while Paper IV relies on values from Degen et al. (2023).

For novel battery materials, due to the unavailability of industrial process data for their production processes, upscaling methods (i.e. empirical factors and process engineering equations) were applied based on small-scale production routes. This includes materials such as conducting redox polymers pEP(QH_2)E and pEP(NQ)E (used as the all-organic battery's electrodes), solid-state electrolytes in ASSBs, and cathode active materials in SIBs. These upscaling methods recalculate the required input materials (such as reagents, solvents, cooling water, and inert gas), input energy, products, emissions, and waste for each production step (Capello et al., 2005; Geisler et al., 2004; Piccinno et al., 2016).

In terms of future battery composition and specific energy, the all-organic battery study considered potential changes in the battery's composition ratio, optimization of the electrode structure, and the corresponding improvements in specific capacity, with inputs from battery researchers (S. Zhang et al., 2022). For ASSBs and SIBs, two simple battery-dimensioning models were developed to estimate the materials and energy required for producing future battery cells, as well as the corresponding specific energy of the battery technologies. These studies considered two battery design scenarios: the "Baseline battery design" and the "Optimal battery design." Further details can be read in Papers III and IV. As a result, four combinations of foreground and background scenarios were explored to assess future changes in the SIB and ASSB systems: 2.5°C - Baseline, 1.5°C - Baseline, 2.5°C - Optimal, and 1.5°C - Optimal.

5. Results and discussions

This section begins by presenting the future environmental performance of studied batteries (Section 5.1): an all-organic battery (Section 5.1.1), two solid-state batteries, (Section 5.1.2), and three sodium-ion batteries (Section 5.1.3) when they are produced at scale, using a functional unit of 1 kWh of energy capacity. Section 5.2 then explores the effects of excluding battery life cycles and other performance parameters in the LCA results. Based on these findings, Section 5.3 outlines strategies for reducing the environmental impacts of studied emerging batteries. Finally, Section 5.4 presents how environmental impacts vary depending on different production scales and discusses the application of LCA across these varying scales.

5.1 Future environmental performance of emerging batteries

5.1.1 Future environmental impacts of an all-organic battery (Based on Paper II).

This section presents the potential environmental impacts of the all-organic battery with considering the upscaling foreground and the advancement in the battery technology. For the selected environmental impact categories, over 91% of the impacts from the all-organic battery production are attributed to the production of electrodes (Table 3), with the cathode (45-66%) showing higher environmental impacts than the anode (33-46%). This disparity is due to the long production route of the cathode backbone, which results in both a high chemical material consumption and high volumes of waste. Among the production stages, the production of electrode backbones contributes the most (60-87%) to the total impacts

(Table 3). Specifically, EDOT, a precursor for electrode backbones, accounts for 21-59% of the impacts in the selected categories.

Table 3. Prospective life cycle assessment characterization results for an all-organic battery and contributions from different production stages to the overall impacts for each impact category using the FU of 1 kWh energy capacity. (Stage I= production of anode backbone, Stage II= production of anode pendant group, Stage III= production of anode, Stage IV= production of cathode backbone, Stage V= production of cathode pendant group, Stage VI= production of cathode, Stage VII = non-electrode component production, Others = Non-electrode components. CC = Climate change, OD = Ozone depletion, HTN = Human toxicity, non-cancer effects, HTC = Human toxicity, cancer effects, IR: Ionizing radiation HH, FE = Freshwater ecotoxicity, MD = Mineral, fossil & renewable resource depletion.)

Impact category	Value (per FU)	Percentage by production stage						
		Anode			Cathode			Others
		Stage I	Stage II	Stage III	Stage IV	Stage V	Stage VI	Stage VII
CC	6.6 x 10^3 kg CO_2-eq	22%	2%	9%	46%	15%	5%	1%
OD	4.3 x 10^{-2} kg CFC-11-eq	26%	1%	20%	42%	0%	2%	9%
HTN	1.4 x 10^{-3} CTUh	27%	2%	6%	48%	11%	3%	2%
HTC	3.9 x 10^{-4} CTUh	21%	3%	9%	45%	16%	5%	1%
IR	5.5 x 10^2 kBq U235-eq	21%	7%	7%	39%	14%	4%	8%
FE	1.7 CTUe	27%	2%	6%	51%	11%	2%	1%
MD	8.1 x 10^{-1} kg Sb-eq	35%	0%	1%	52%	11%	1%	0%

Solvents, particularly trichloromethane used in the production of the EDOT precursor, are significant contributors to ozone depletion (89%) and climate change (16%), human toxicity with (12%) and without (14%) cancer effects, freshwater ecotoxicity (12%), and ionizing radiation (9%) (Figure 5). Catalysts (e.g. NH_3Cl/Zn, CuO) predominantly contribute to resource depletion (88%), human toxicity non-cancer effects (29%), and freshwater ecotoxicity (32%). Waste treatment processes emit significant amounts of

GHGs and toxic chemicals, thus contributing considerably to global warming potential (37%) and human toxicity, with (53%) and without (15%) cancer effects. They also significantly impact freshwater ecotoxicity (13%) and ionizing radiation (6%). Energy usage, particularly from nuclear-based electricity production using uranium, is a major contributor to ionizing radiation (50%) and a significant source of climate change impact (15%). Bromine production, used in various production stages, is another individual contributor for climate change (10%), human toxicity with (4%) and without cancer effect (8%), ionizing radiation (6%), and freshwater toxicity (6%).

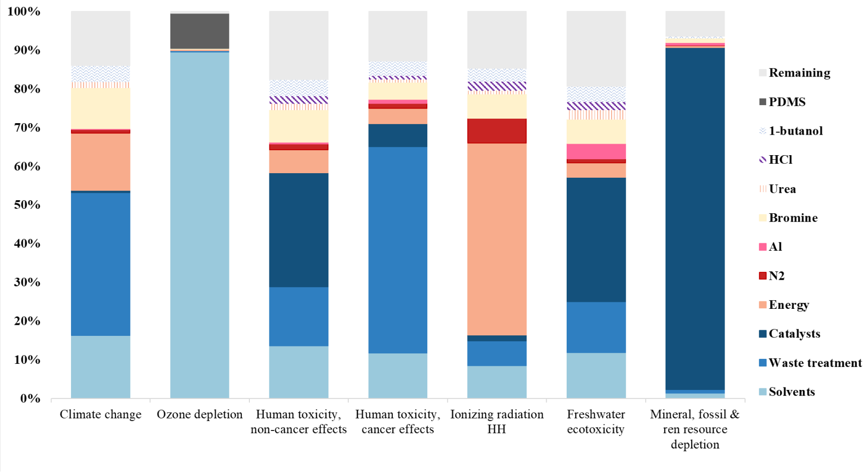

Figure 5. Relative contribution of different process flows in large-scale production of the all-organic battery to the most significant impact categories.

In comparison to the flexible LIB (Figure 6), the all-organic battery exhibits higher environmental impacts in most categories, except for ionizing radiation. The flexible LIB exhibits high ionizing radiation impacts due to the substantial electricity consumption in the production of carbon nanotube current collectors. Swedish electricity mixture is used in the manufacturing process, which is characterized by a high proportion of nuclear energy. The use of uranium in nuclear energy production is a large contributor to the ionizing radiation impact, as mentioned in the previous paragraph. Besides the long synthesis route of electrodes production, the overall higher environmental impacts of the organic battery are also linked to its relatively low specific energy (21.6 Wh/kg), which is five times lower than that of the flexible Li-ion battery (108 Wh/kg).

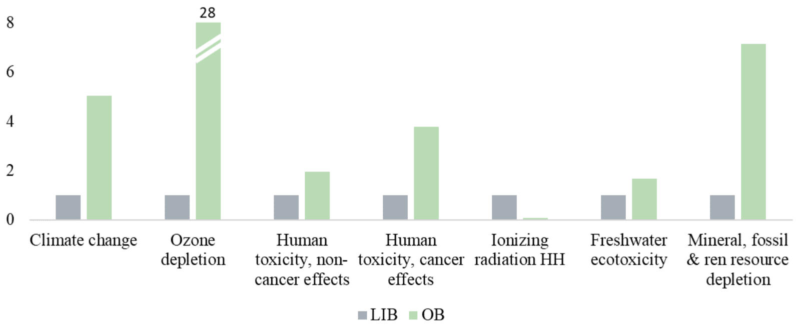

Figure 6. Comparison of the environmental performance of the all-organic battery and the flexible LIB. Normalized to the impact of LIB, where LIB is 1.

5.1.2 Future climate impact of all-solid-state batteries (Paper IV).

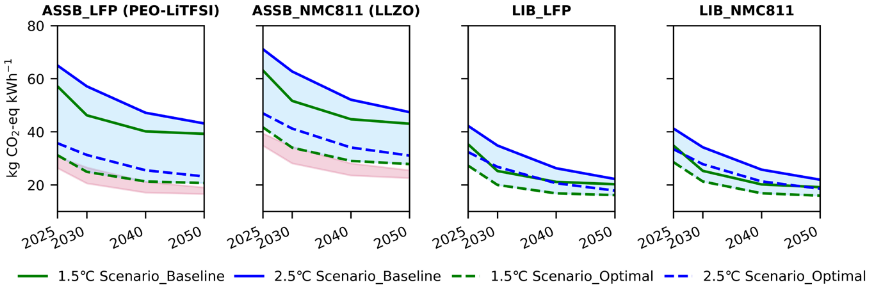

Figure 7. Climate impact results per kWh of battery capacity for studied all-solid-state batteries at different years under four distinctive scenarios. The shaded blue area illustrates the disparity in climate impact resulting from different scenarios. The shaded pink area illustrates the climate impact of ASSBs under the best battery design scenario (i.e. using an extra thin electrolyte layer).

Overall, ASSBs exhibit a higher climate impact than their LIB counterparts with the same cathode active materials across different years and scenarios (Figure 7). A review study found that GHG emissions from ASSBs are generally higher compared to LIBs, and these were explained because of the early development stages of ASSB technologies (Mandade et al., 2023).

In 2025, the climate impact of studied ASSBs and LIBs is lower compared to previous LCA studies (Kallitsis et al., 2024; Mandade et al., 2023). This can be attributed to variations in battery design, battery specific energy, production region, use of secondary materials, and the incorporation of future decarbonization strategies. Notably, only one LCA study has been conducted on polymer-based electrolyte ASSBs (Vandepaer et al., 2017). This study employs LFP as the cathode and Li as the anode, but the composition of the electrolyte material and the relevant production processes remain undisclosed due to the use of confidential industrial data. The results indicate GHG emissions ranging from 70-98 kg CO_2-eq/kWh (Vandepaer et al., 2017), which are up to 3.2 times higher than those observed in this study (Paper IV). For ASSBs with LLZO electrolytes, a pioneering study by Troy et al. (2016) reported GHG emissions of 1045 kg CO_2-eq/kWh for batteries using an LCO cathode and Li anode, which is up to 23 times higher than the climate impact of our ASSB NMC811 (LLZO) in 2025. Their high climate impact was primarily due to the non-optimized battery design, which led to the excessive use of non-active materials with high GHG emissions, and low battery specific energy. Furthermore, using LCO as cathode active materials also contribute to the low specific energy of their battery. In a recent study, Liu et al. (2024) analyzed an ASSB cell with a specific energy of 310 Wh/kg that includes a LFP cathode, Li anode and LLZO electrolyte, reporting a climate impact of approximately 133 kg CO_2-eq/kWh.

From 2025 to 2050, the climate impact of ASSBs and LIBs shows a significant reduction. Specifically, the climate impact decreased from 31-65 kg to 21-43 kg CO_2-eq/FU for ASSB LFP (PEO-LiTFSI), from 42-71 kg to 28-47 kg CO_2-eq/FU for ASSB NMC811 (LLZO), from 27-42 kg to 16-22 kg CO_2-eq/FU for LIB LFP, and from 29-41 kg to 16-22 kg CO_2-eq/FU for LIB NMC811. These reductions correspond to a decrease in climate impact of 31-35% for ASSB LFP, 32-34% for ASSB NMC811, 41-47% for LIB LFP, and 44-47% for LIB NMC811 from their respective 2025 levels. This trend is consistent with findings from other LCA studies using similar methodologies (Xu et al., 2022; Zhang et al., 2024). These reductions can be attributed to the decarbonization of the energy sector, the integration of carbon capture and storage (CCS) technologies in industrial power and heat generation, and the increased use of secondary materials in battery production. The REMIND model indicates a significant increase in the share of renewable resources in European electricity generation, rising from 58% to 96% (between 2025 and 2050), and from 67% to 97% (between 2025 and 2050) under the 2.5°C and 1.5°C scenarios, respectively. Accordingly, the climate impact of the European medium voltage electricity mix is estimated to drop from 107-157 g CO_2-eq/kWh in 2025 to 13.6-22 g CO_2-eq/kWh by 2050. It is important to note that these climate impact reductions of studied batteries between 2025 and 2050 are not influenced by the battery design, since the battery design does not change overtime in the model.

When assessing the impacts of various scenarios on the studied batteries for a given year (as indicated by the shaded blue area in Figure 7), it reveals that disparities in the climate impact for ASSBs are mainly influenced by the battery design. Optimizing the battery design could reduce climate impact by 45-47% for ASSB LFP (PEO-LiTFSI), 34-35% for ASSB NMC811 (LLZO), 20-23% for LIB LFP, and 15-19% for LIB NMC811, regardless of the production year and climate scenarios. Additionally, stronger climate targets (1.5 °C scenarios) and increased secondary material content would reduce the climate impact by 9-20% for ASSB LFP (PEO-LiTFSI), 9-18% for ASSB NMC811 (LLZO), 9-27% for LIB LFP, and 13-26% for LIB NMC811. These findings demonstrate that, for ASSBs, optimizing battery design is more efficient for reducing the climate impact compared to implementing stricter climate and mineral recirculate policies. This does not apply to LIBs, as their design is relatively mature and has almost approached its limit for further improvement, which highlights the importance of design improvements on their environmental performance in the early stages of battery technology development.

Comparing the optimal battery design to the baseline battery design, the battery specific energy increased 60% for ASSB LFP (PEO-LiTFSI) and 47% for ASSB NMC811 (LLZO). In the baseline design scenario, the ASSBs' specific energy values fall below market expectations, while in the optimal design scenario they meet the projected expectations. Previous studies have discussed that the market expects a minimum specific energy requirement of 350 Wh/kg for the first generation of commercial ASSB(Frith et al., 2023; Schmaltz et al., 2022; Tian et al., 2021), with the potential for surpassing this number in future designs (Randau et al., 2020). This suggests that the climate impact of ASSBs is more likely to fall into the lower range and has the potential to be reduced beyond the values reported in this study.

It is also important to note that the parameters employed in the optimal design scenario represent potential achievable designs under current technological conditions rather than the performance limits of these battery technologies. By reducing the electrolyte layer thickness to reported minimal values (20 μm for LLZO and 25 μm for polymer-based electrolytes) (Kravchyk et al., 2021; Lennartz et al., 2023), while simultaneously keeping other parameters constant, our model suggests that the climate impact of

ASSBs could be reduced to levels comparable to LIBs, but not lower, as illustrated by the pink area in Figure 7.

The solid electrolytes, PEO-LiTFSI and LLZO, are the primary contributors to the climate impact of ASSBs, accounting for 28-55% of the total impact for ASSB LFP and 48-67% for ASSB NMC811 across all production years and scenarios. These findings are consistent with previous LCAs on ASSBs (Mandade et al., 2023). The high GHG emissions associated with these electrolytes stem from their high production emissions (kg CO_2-eq/kg) and the large quantities (kg) used in the batteries. In PEO-LiTFSI production, LiTFSI is the principal source of GHG emissions, contributing up to 84% of PEO-LiTFSI's impact. Although LiTFSI is widely used in PEO-based polymer electrolytes, due to its ease of dissolution and good ionic conductivity, it is not indispensable. Alternative electrolyte salts could be explored to reduce the climate impact. For example, Wickerts et al. (2023) showed that replacing LiTFSI in lithium-sulfur batteries could reduce the climate impact of the battery by 60%. This indicates that ASSB LFP (PEO-LiTFSI) has the potential for further impact reduction, however, this will require additional research. For LLZO, lanthanum oxide production is the main contributor, accounting for up to 90% of the LLZO’s emissions, due to significant inputs from precursor materials such as citric acid, ammonium sulfate, and ammonium bicarbonate.

Cathode active materials also play a crucial role, contributing 13-26% of the total impact for ASSB LFP (PEO-LiTFSI) and 19-36% for ASSB NMC811 (LLZO). Their impact is even greater in LIBs, in which they contribute 24-37% for LIB LFP and 48-63% for LIB NMC811. The high impact of cathode active material NMC811 is associated with the extraction of minerals and processing of materials such as nickel sulfate, cobalt sulfate, lithium hydroxide, as discussed in a previous study (Xu et al., 2022). Li foil, serving as the anode in ASSBs, represents 14-27% of the total climate impact for ASSB LFP (PEO-LiTFSI) and 3-10% for ASSB NMC811 (LLZO). Battery manufacturing energy usage contributes 3-7% of total ASSBs emissions, varying by year and scenario, but has a more substantial role in LIBs, particularly for LIB LFP, where it constitutes 14-27% of its total emissions. The Al current collector contributes 9-12% to ASSB LFP (PEO-LiTFSI) emissions but only 3-4% to ASSB NMC811 (LLZO).

5.1.3 Future climate impact of sodium-ion batteries (Based on Paper III).

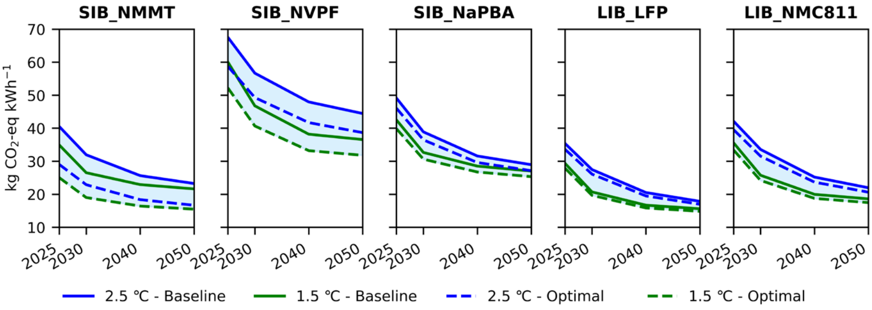

Figure 8. Climate impact results per kWh of battery capacity for studied sodium-ion batteries and lithium-ion batteries at different years under four distinctive scenarios. The shaded blue area illustrates the disparity in climate impact resulting from different scenarios.

Overall, NMMT exhibits the best performance among the three studied SIBs, with climate impact comparable to those of LIBs (Figure 8). NaPBA shows higher climate impact than LIBs, while NVPF demonstrates the highest emissions among SIBs. Such disparities in climate impact arise from differences in the materials that are used in each battery type. Different materials have varying energy consumption requirements and emissions during production, which in turn affect the overall climate impact (Peters et al., 2021). Additionally, the choice of battery material influences the energy capacity of the battery, further affecting the climate impact per unit of energy stored. A recent prospective LCA study on various sodium battery technologies reported emissions that were several times higher than those in our study when using the same functional unit (Lai et al., 2023). Such a notable difference may due to the high emission electricity grid that they use in the mode (Chinese electricity mixtures), coupled with the exclusion of considering potential future changes in the background system.

From 2025 to 2050, the climate impact of all studied batteries are decreasing, similar to the trend observed in the ASSB results (Paper IV). NMMT's climate impact decreased by 38-43%, from 25-41 to 15-23 kg CO_2-eq/FU. NVPF's impact decreased by 34-39%, from 52-68 kg to 32-44 kg CO_2-eq/FU. NaPBA shows a reduction of 36-41%, from 40-49 kg to 25-29 kg CO_2-eq/FU. LFP's impact decreased by 47-50%, from 28-35 kg to 15-18 kg CO_2-eq/FU, while the climate impact of NMC811 decreased by 47.7-47.9%, from 33-42 kg to 17-22 kg CO_2-eq/FU. As discussed in ASSB study

(Paper IV), these reductions are primarily driven by the increased integration of renewable energy into the electricity grid, the implementation of carbon capture and storage (CCS) technologies in industrial processes, and the use of secondary materials.

Unlike the ASSB study (Paper IV; which considers the potential optimization of battery composition through changing the thickness of battery components), the optimal performance scenario in the SIB study focuses on potential changes in cathode usable capacity. Based on the results shown in Figure 8, improving battery performance can significantly reduce the climate impact of SIBs.

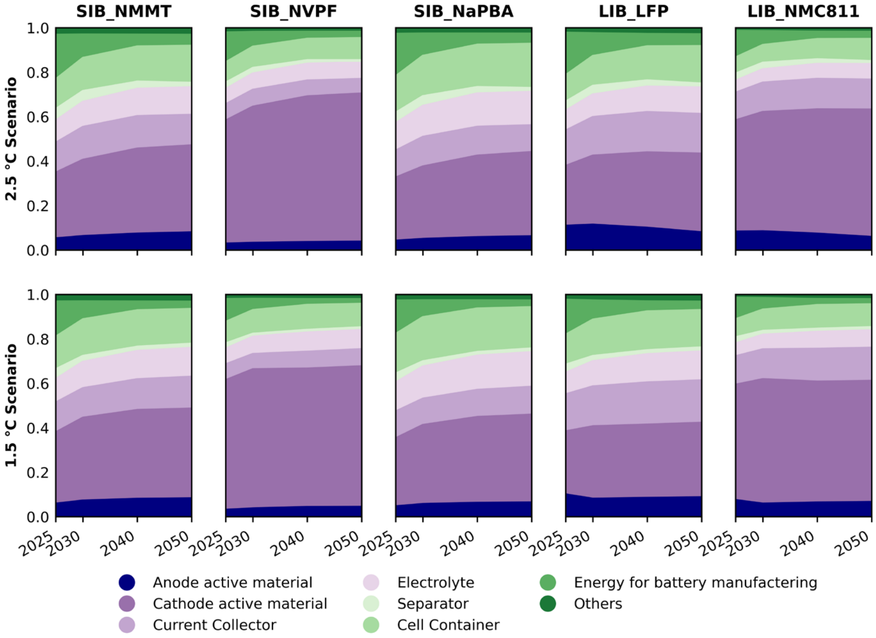

Figure 9. Relative contributions to overall climate impact of sodium-ion batteries and lithium-ion batteries.

Cathode materials emerge as key contributors to the climate impact across all battery types (Figure 9), primarily due to the energy-intensive processes involved in mineral mining, processing, and high-emission production methods such as hydrogen cyanide production, as well as the high proportion (wt.%) of cathode active material in the battery cell. Specifically, cathode active materials contribute 30-40% of the total climate impact in NMMT, 55-67% in NVPF, 28-39% in NaPBA, 27-35% in LFP, and 50-57% in

NMC811, regardless of the production year or applied scenarios. The cathode active material plays a significant role in NVPF battery, due to the production of precursor material V_2O_5, which is a precursor material modeled as a by-product of primary steel production. The climate impact of V_2O_5 production was calculated based on economic allocation. It needs to be noted that the choice of allocation methods can significantly influence the climate impacts results (Paper III).

Energy consumption during battery manufacturing also plays a significant role in the overall climate impact (Figure 9). Reductions in energy consumption emissions from the manufacturing process have contributed substantially to the overall decrease in climate impact from 2025 to 2050. The cell container, with steel as the primary material, accounts for 13-17% of the total climate impact in NMMT, 9-10% in NVPF, and 16-20% in NaPBA. The current collector (Al foil) contributes 13-15% in NMMT, 7-8% in NVPF, and 12-13% in NaPBA. The electrolyte also represents a significant portion of the climate impact, contributing 10-13% in NMMT, 7-9% in NVPF, and 12-16% in NaPBA. This is because of the high production emissions associated with sodium hexafluorophosphate ($NaPF_6$), which range from 12-17 kg CO_2-eq/kg, regardless of the production year or scenario.

5.2 Impact of excluding key battery performance parameters

Considering battery performance parameters such as lifetime, discharge depth, and round trip-efficiency in the functional unit could provide a more realistic projection of the environmental performance of future batteries. A commonly used functional unit for incorporating these additional parameters is 1 kWh of electricity delivered over battery's lifetime. Previous studies have shown that these factors can significantly affect the environmental impacts of batteries (Peters et al., 2017; Vaalma et al., 2018). These parameters can be particularly important for novel battery chemistries, which often displays different aging mechanisms compared to their LIB counterparts. However, obtaining or estimating such data for emerging batteries, particularly those with low TRL like the all-organic battery in Paper I&II and ASSBs in Paper IV, remains challenging. This section provides a general discussion on these considerations.

In the all-organic battery study (Papers I and II), lab experiments demonstrated that the battery could retain 85% of its initial capacity after 500 charge-discharge cycles. Battery experts have suggested that the cycle life could be improved in the future, although specific figures are not yet available. In contrast, the reference flexible battery system is based on the LCO/LTO chemistries. The LCO/LTO system typically displays very long cycle life in commercial LIBs. For example, a conventionally designed LCO/LTO battery system has been reported to achieve a lifetime of 4000 cycles (Majima et al., 2001). For the all-organic battery to have comparable environmental impacts to the flexible LIB system, it would need to exceed this 4000-cycle lifespan due to the inferior environmental performance of the all-organic battery, as discussed earlier. Considering its expected application in wearable devices with a lifespan of less than five years (approximately 1825 charge-discharge cycles assuming daily charging), it is unlikely that the all-organic battery could outperform the flexible LIB in environmental performance given the practical lifespan limitations.

In the ASSBs study (Paper IV), solid-state electrolytes can withstand higher temperatures than liquid electrolytes, reducing degradation mechanisms such as electrolyte decomposition, electrode dissolution, and possibly side reactions. This characteristic could theoretically lead to batteries with a reduced capacity to fade over multiple charge-discharge cycles, resulting in longer-lasting batteries. However, opinions vary on this aspect. A market report suggests that ASSBs could maintain 90% of their capacity after 5000 cycles (Crawford, 2022). Nevertheless, battery experts on the author team are more sceptical due to the issues related to their energy efficiency, Coulombic efficiency, as well as the fragility of solid parts under harsh operation conditions and especially vibrations (Paper IV). A rough calculation indicates that for ASSB LFP and ASSB NMC811 to achieve better climate impact performances than LIB LFP and LIB NMC811 in 2025, their lifetimes would need to be approximately 1.5 and 1.7 times longer, respectively. This analysis based on the climate impact values projected for 2025 with 2.5°C-baseline scenario.

More data available for the SIBs, due to their relatively high TRL. Consequently, data on discharge depth, battery cycle life, roundtrip efficiency were collected (Zhang et al., 2024) (Paper III). The results indicate that, when considering factors such as lifetime, depth of discharge, and round-trip efficiency, the three studied SIBs can outperform LIB NMC811 under the best performance scenario, while also showing comparable emissions to LIB LFP (Figure 10).

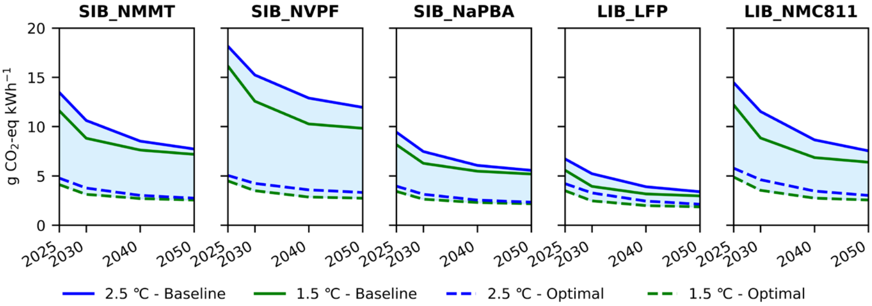

Figure 10. Climate impact results of studied SIBs at different years, under four scenarios. Results are expressed per kWh of electricity delivered along lifetime. The shaded blue area illustrates the disparity in climate impact resulting from baseline and optimal performance scenarios.

5.3 Opportunities for mitigating environmental impacts (Paper II-IV)

Improving the environmental performance of emerging batteries requires a collective effort across multiple sectors along the production chain. In general, strategies for environmental impact mitigation can be categorized into three key areas: battery technology, novel battery material production processes, and background material production processes.

At the battery technology level, efforts to reduce environmental impacts should be focused on optimizing composition and performance (S. Zhang et al., 2022; Zhang et al., 2024). This includes increasing the proportion (wt.%) of active materials, such as enhancing the cathode's mass loading (mg/cm^2), and minimizing the proportion of other components, including the electrolyte, anode, current collector, and cell casing. Additionally, improving the usable cathode specific capacity (mAh/g), extending battery life, and increasing energy efficiency are crucial actions for minimizing the environmental footprint.

At the production process level, particularly for novel battery materials with high environmental impacts, optimizing synthesis routes is essential. This can involve the replacement of materials with significant environmental impacts, simplifying synthesis route to reduce material and energy use, and exploring more environmentally friendly synthesis routes(S. Zhang et al., 2022).

For background production processes, increasing the share of renewable energy in the power grid and steel industries, as well as implementing carbon capture and storage (CCS) technologies, are necessary steps for reducing GHG emissions that are associated with battery production. To achieve these improvements will require coordinated efforts not only from battery manufacturers but also from all sectors involved in the battery production chain, including electricity, heat and power, and steel(Zhang et al., 2024). Future battery or component factories could also consider locating near clean energy sources such as hydropower, wind, or solar energy to further mitigate emissions (Zhang et al., 2024). Furthermore, policy and regulatory measures play a pivotal role in advancing sustainable battery production. Existing regulations on the recycled content of critical materials may need to be more specific, for example, regarding rare earth elements used in ASSBs. Indeed, policies that incentivize the use of renewable energy and enforce stricter emissions standards can propel the industry towards more sustainable practices (Paper IV).

5.4 Comparison of lab-scale and industrial-scale LCA for an all-organic battery: interpretations and insights (Paper I-II)

This section presents the lab-scale LCA results for the all-organic battery and compares them to the industrial-scale LCA results. Based on the results (Papers I and II), a discussion on the application of different scales of LCA and how to best interpret these results is performed.

The lab-scale LCA results show that electrodes are the dominant contributors to environmental impact, accounting for more than 99% of the total impact across all selected categories, with the cathode having a greater impact than the anode (Paper I). This is largely a result of the extensive synthesis process that is required for electrode materials, particularly for the cathode backbone structure.

Figure 11 a) summarizes the key individual contributors to various impact categories. For mineral, fossil, and renewable resource depletion, the greatest contributors are catalysts and solvents. Specifically, the production of $Pd(PPh_3)_4$, which was used as a catalyst in synthesizing the electrode backbone EP(OH)E, is responsible for 66% of the total resource depletion.

In other impact categories, solvent use emerges as the primary contributor, responsible for 59–99.7% of the total impact. Additionally, waste treatment plays a significant role in climate impact (37%), human toxicity (15% for cancer and 20% for non-cancer effects), and freshwater ecotoxicity (27%). Notably, there is a positive correlation between solvent use and the amount of waste generated, meaning that increased solvent use leads to more waste that requires treatment.

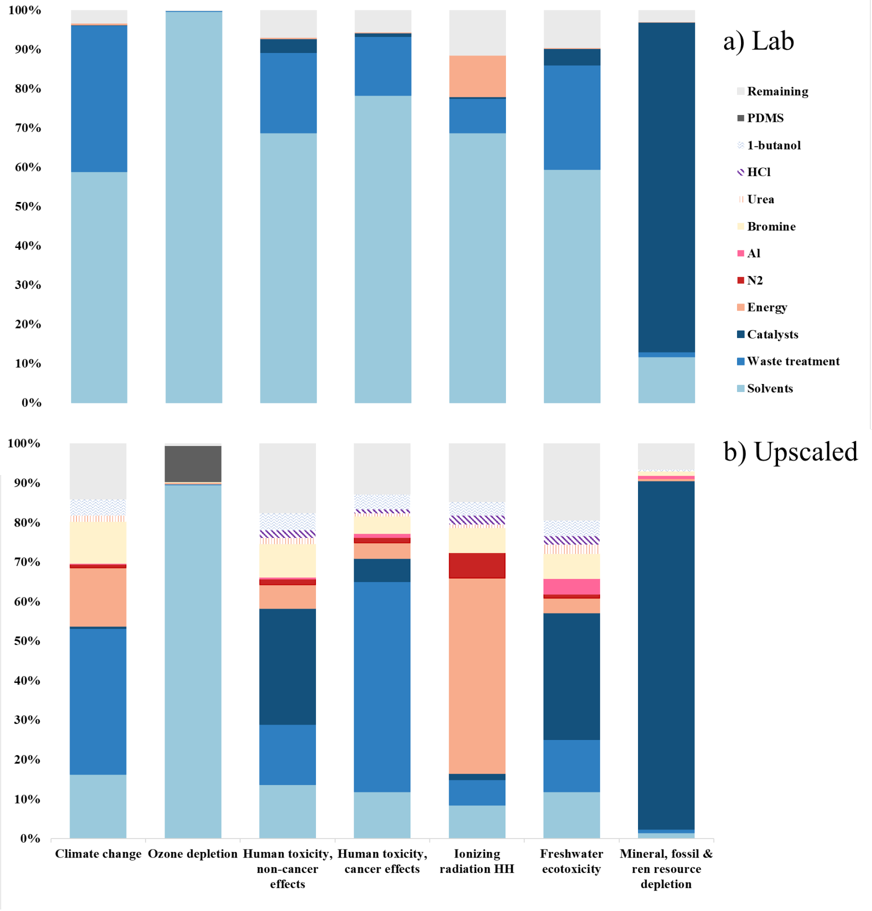

Figure 11. Environmental hotspots of the all-organic battery resulted from lab-scale LCA (a), and industrial-scale LCA (b). Note: panel b) is the identical to Figure 6, included here for easier comparison.

The transition from lab-scale to industrial-scale shows a 97-99% reduction in environmental impacts across selected impact categories, driven by increased efficiency in material use (such as solvents, catalysts), reduced waste, and optimized battery composition and performance. As a result, environmental hotspots have shifted, and new hotspots have been uncovered, as shown in Figure 11. Specifically, improvements in solvent use efficiency is the primary contributor to the total reductions across various impacts categories (59–99.8%), except for resource depletion potential, where it contributes only 9% of the reduction. Additionally, reducing the use of zinc and palladium (Pd) catalysts reduces resource depletion, contributing to 14% and 75% of the reduction, respectively. Previous studies suggest that environmental impacts tend to decrease as production scales up and technologies mature. This trend can be attributed to enhanced material and energy efficiencies and the increased solvent recycling and waste reduction. For example, Gavankar et al. (2015) found that scaling up production could reduce the environmental impacts of carbon nanotubes by 84-94%, while Piccinno et al. (2015) reported that upscaling nano-cellulose production from lab to industrial scale could decrease environmental impacts by up to 85%.

The differences observed between lab-scale and large-scale LCA results highlight the importance of applying lab-scale LCAs results with caution and clearly communicating their scope. It is evident that lab-scale LCAs cannot represent the environmental performance of batteries at an industrial scale for long-term decision-making. Rather, lab-scale LCAs provide an initial screening of the environmental impacts of emerging batteries, identifying significant environmental hotspots, such as the extensive use of materials or energy-intensive steps in the synthesis process. By recognizing these inefficient processes, stakeholders, such as chemical and process engineers, can focus on optimizing these steps as the technology scales. This may involve shortening synthesis routes, reducing solvent use, developing efficient catalysts, or finding alternative input materials that are better suited for large-scale production. Moreover, lab-scale LCA results can inform chemical engineers about adopting more sustainable laboratory practices. The insights gained from these assessments also serve as a crucial foundation for conducting prospective LCAs, thus enabling a focus on key environmental hotspots during the scenario development phase of pLCA.

Lab-scale LCA results can also be used for a quick and preliminary assessment of the environmental performance of upscaled emerging systems by discussing potential changes in key environmental contributors during the transition from laboratory to industrial scales. This may require the engagement of stakeholders such as process engineers who have expertise in scaling up. Process flows that often experience significant reductions during upscaling should be discussed, such as solvents (Pallas et al., 2020b; Piccinno et al., 2018), energy (Gavankar et al., 2015; Piccinno et al., 2015), and materials that are likely to be recycled in mass production, e.g., metals (Pallas et al., 2020a, 2020b; Villares et al., 2017).

Different methods are suited to different research questions, and no single method is universally superior to others (Guinée et al., 2018). Lab-scale LCA provides a detailed snapshot of immediate environmental impacts based on current technology and production systems. On the other hand, industrial-scale LCA gives insights into the potential longer-term impacts at full production capacity. Both levels of analysis highlight the continuous need for advancements in processes to mitigate significant environmental impacts of the all-organic battery. The dynamic nature of these assessments emphasizes the importance of incorporating lifecycle thinking throughout the development process of the battery product to guide technological innovations towards a more environmentally friendly direction.

6. General discussion

Methodological limitations in impact categories coverage

ASSBs (Paper IV) and SIBs (Paper III) studies focus particularly on the climate impact, due to the inherent limitations within integrated assessment models (IAMs). IAMs offer detailed representations of sectors that are critical to climate change but they often lack coverage in areas such as agriculture and chemical production (Pauliuk et al., 2017). Consequently, the pLCA databases derived from IAM outcomes do not capture potential changes in other impact categories. This indicates a need for further developing pLCA databases.

Methodological limitations in upscaling method

The upscaling of chemical processes in this study assumed that the industrial production route would remain the same as the small-scale synthesis route. This assumption implies that the types of reagents, energy, solvents, and catalysts used at the industrial scale would be identical to those used in the small-scale. However, the quantities of these materials were recalculated for industrial scale using empirical parameters and process design equations for each reaction step. This assumption might be more justified for novel materials with a TRL of 5 or higher, where the production processes have been validated at an engineering scale in a relevant environment. For materials at a lab scale (TRL < 5), the synthesis pathways and input materials are likely to undergo further optimization.

In practice, the synthesis route typically evolves through different stages of TRL development as new chemical progresses. Early-stage research often prioritizes scientific feasibility over practical applications (S. Zhang et al., 2022). As the TRL advances, factors like scalability, cost, safety, and environmental impact gain importance, leading to modifications and optimizations of the synthesis route. This could include eliminating inefficient steps, substituting input materials for more cost-effective or accessible alternatives, and recirculating solvents. By the time a process reaches a higher TRL, it usually has been refined several times to satisfy large-scale production requirements (Weyand et al., 2023). Consequently, the final industrial production route and the input materials can significantly differ from those at the lab-scale (Weyand et al., 2023). Therefore, synthesis routes developed in the early stages may not accurately represent those used at industrial scale. Thus, applying upscaling methods to these systems and using the results to represent future industrial processes may lead to high uncertainties.

Methodological insights gained from the thesis

There is currently no established framework or guidance for conducting LCA on emerging battery technologies. Drawing on the insights gained from Papers I-IV, this thesis offers some insights that may be valuable for future studies. It is crucial, in the goal and scope definition of the LCA, to evaluate the TRLs not only of the overall battery technology but also of its individual components (S. Zhang et al., 2022), as outlined in Table 2. For batteries using novel chemicals at a TRL below 5 (lab-scale), it is recommended to conduct an LCA based on laboratory processes, complemented by a pLCA for the potential upscaled system. As previously discussed, at this early stage, the production system is expected to undergo significant modifications as it develops toward industrial-scale manufacturing. Therefore, at this stage, the LCA primarily provides short-term guidance for chemical engineers, assisting in the sustainable development of these processes.

For emerging batteries where more information is available (often with a TRL of 5 or higher for both technology and materials), this information provides a more solid foundation for conducting a pLCA with a long-term focus. When performing a pLCA, it is critical to consider potential changes in three key areas: the composition and performance of the battery technology, the foreground system (battery manufacturing and novel material production), and the background system (remaining energy and material production processes).

Conducting a LCA on emerging battery technologies also requires the engagement of relevant stakeholders, including chemical engineers, battery developers, and process engineers, who play different roles across the battery value chain and development stages. Chemical engineers focus on developing new materials to enhance battery performance. Battery developers focuses on how to integrate these novel materials into battery systems. Process engineers are vital during the scale-up and manufacturing phases, where they optimize production processes, address engineer challenges related to mass production, and improve efficiency. Therefore, their involvement can help LCA practitioners to understand current material synthesis. Additionally, stakeholder engagement can assist validate the assumptions made in large-scale production processes and battery composition and performance. In such an interdisciplinary collaboration, LCA practitioners must have basic knowledge of the battery technology, including its working principles and production processes. This foundational knowledge ensures a shared understanding and enhances collaboration. To effectively obtaining relevant information from these collaborators, it is important to clearly outline the data required for LCA and communicate how this data will be used. At the early stage of the collaboration, offering some preliminary results based on the best available data can help engage stakeholders and facilitate their understanding of how specific data points influence the overall outcomes.

Data contribution regarding the battery technologies

Data on battery composition and corresponding battery performance (e.g. specific energy and energy density) is often lacking, especially for emerging batteries. SIBs (Papers III) and ASSBs (Paper IV) studies address this by developing two simple models to estimate the required data. These two models enable fair comparisons among studied batteries by standardizing battery dimensions and design assumptions. It also links the amount of material used to the resulting battery performance (i.e. specific energy and energy density), enhancing the consistency of the dataset. Additionally, the model offers flexibility in adjusting the battery design, allowing for the exploration of different design scenarios. The models developed in Paper III and IV, as well as the development framework, can be used for future studies.

The battery dimensioning models begins by identifying the intended use of the battery. Based on the battery chemistry and application requirements, the size and shape of the battery cell are determined, such as selecting a pouch cell for ASSBs and a thin film for flexible batteries. Internal design features, such as using single- or double-side electrode coatings or a bipolar configuration, should be determined and used consistently. Using available data reported from battery studies or estimates from battery researchers, such as mass loading (mg/cm^2), areal capacity (mAh/cm^2), and electrode mixture thickness, combined with the density and porosity of the electrode mixture, the weight ratio of each electrode material, as well as the battery’s dimension, allowing us to calculate the required amount of each electrode material. The quantities of other battery materials are then calculated based on the their material density and estimated thickness, and battery’s dimensions. By summing the materials calculated in the previous steps, the total battery mass is obtained. The battery capacity (mAh) can be estimated using the cathode active material's capacity (mAh/g) and its amount. Finally, the specific energy (Wh/kg) and volumetric energy density (Wh/L) of the battery cell are calculated based on the battery capacity, voltage, and the total battery mass and volume.

7. Conclusion

Based on a functional unit of 1 kWh of battery capacity, the all-organic battery was found to have higher environmental impacts compared to LIBs, mainly due to their low specific energy and inefficient synthesis routes required for electrodes production. The ASSB with NMC811 and LLZO electrolyte has a higher climate impact compared to the LIB with NMC811. The ASSB with LFP and a polymer electrolyte has the potential to achieve a climate impact comparable to the LIB with LFP, under the best battery design scenario. For SIBs, NMMT type with optimized battery performance scenarios showed climate impact comparable to those of LIBs, while NVPF and NaPBA exhibited higher impacts.

Key findings in this thesis indicate that for the all-organic battery, the electrodes, particularly the cathode backbone, are the main contributors to environmental impacts at both lab and industrial production scales. This is largely due to the long synthesis route of the cathode backbone, which requires substantial material consumption. Key contributors include the precursor chemical EDOT, catalysts, and solvents like dichloromethane. For the studied ASSBs, the solid-state electrolyte and cathode active materials are the primary contributors to climate impact for both LLZO-based and polymer-based ASSB, with the anode and current collector also being significant in the polymer-based ASSB. In the case of SIBs, the cathode is a key contributor across three studied SIBs, with the current collector, electrolyte, and cell casing also being significant in NVPF and NaPBA.

Notably, transitioning from lab-scale to large-scale production could reduce the environmental impact of the all-organic battery by up to 99%, mainly through optimized material use and recirculate solvents. This underscores the importance of clearly defining lab-scale LCA objectives and carefully interpreting the results. Lab-scale LCAs offer valuable early insights, which enables chemical engineers to adjust synthesis routes. This approach is especially well-suited to emerging batteries with low TRL in both technology and materials.

Strategies for reducing the environmental impacts of the studied emerging batteries include improving battery composition and performance, increasing the use of recycled materials, and implementing decarbonisation efforts in energy intensive upstream and downstream production processes. These efforts could involve integrating more renewable energy sources into the electricity system and adopting carbon capture and storage technologies.

8. Future research

Addressing supply chain resilience

Before scaling up battery technologies, it is important to quantify material demands and assess the resilience of the supply chain. This analysis can provide insights into the potential impacts of upscaling up on the existing supply chain, helping to identify and evaluate risks such as potential mineral supply bottlenecks. Preliminary calculations from the ASSB study (Paper IV) suggest that the lanthanum needed to produce ASSBs between 2030 and 2035 could be 166 times the current annual global production. In contrast, the SIBs study (Paper III) shows the potential of SIBs to reduce pressures on critical mineral resources. These findings highlight the need for a more thorough assessment to support informed decision-making.

Expanding the scope for additional environmental impact categories and other sustainability perspectives

While this thesis focused on the climate impact perspective in the ASSB (Paper IV) and SIB (Paper III) studies, future research should expand its scope to include other environmental impact categories. This will provide a more comprehensive understanding of the environmental performance of these emerging batteries and help prevent potential environmental burden shifting. Additionally, future study can also consider perspectives such as economic cost, social impacts, technology performance, and safety when evaluating the sustainability of emerging batteries.

Considering battery end-of-life and recycling

The end-of-life treatment of batteries is a critical area that requires further exploration as more data becomes available. Current challenges include the low economic viability of recycling due to the absence of valuable minerals in some batteries and the technical difficulties posed by diverse battery chemistries (Cui and Zhang, 2008; Morse, 2021; Yao et al., 2018). As recycling technologies advance and recycling regulations evolve globally, it will become increasingly feasible and important to broaden the scope of LCA studies to include the battery's reuse and recycling stage. This expansion is likely to affect the comparison between emerging batteries and LIBs, and provide a more comprehensive understanding of the environmental performance of these emerging technologies.

Engaging stakeholders and interdisciplinary collaboration

Conducting life cycle assessments, especially prospective ones, requires knowledge from various fields. Future studies should consider and prioritize stakeholder engagement from the initial stages of the research process. When applying for research grants, it is crucial to build partnerships and secure funding that supports the involvement of diverse expertise.

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Popular science summary

Batteries are essential to our modern lives, powering everything from smartphones to electric vehicles. As we move towards a more sustainable future, the demand for advanced batteries is growing rapidly. Imagine batteries that are flexible and bendable, capable of powering wearable devices to monitor our health in real time; batteries that can power cars for long distances without needing frequent recharging; and batteries that are affordable, making electric vehicles accessible to everyone. These demands are driving the development of new batteries such as flexible all-organic batteries, all-solid-state batteries (ASSBs), and sodium-ion batteries (SIBs). Before these new batteries reach the market, it is crucial to understand their environmental impact, which is the focus of this thesis. This thesis work explores the environmental performance of a flexible all-organic battery, two ASSBs, and three SIBs, comparing them to traditional lithium-ion batteries (LIBs) using life cycle assessment (LCA) and prospective LCA.

Key Findings:

- The all-organic battery was found to have higher environmental impacts than LIBs because it stores less energy per mass, meaning more batteries are needed to do the same job, leading to more emissions during production. The cathode materials, in particular, contribute significantly to these impacts due to their resource-intensive production processes.

- ASSBs showed higher or comparable climate impact than LIBs, primarily because of the high emissions associated with producing solid electrolytes and cathode active materials.

- SIBs vary in their environmental impacts, with the layered oxide type showing similar climate impact to LIBs, while others showing higher climate impact than LIBs. The cathode is the biggest contributor for all three types of SIBs.

It's important to note that these comparisons focus only on the production process. When considering the battery's use phase and end-of-life, the results may change.

What can be done: Despite these challenges, we may still want these advanced batteries on the market due to the function they offer. Therefore, how can we improve their environmental performance? The studies suggest that by optimizing battery designs, using more clean electricity in manufacturing processes, and using more recycled materials, we can significantly reduce their environmental footprint.

The research in this thesis provides valuable insights for battery developers, helping them create more environmentally friendly batteries that will support our transition to a sustainable future.

Populärvetenskaplig sammanfattning

Batterier är oumbärliga i våra moderna liv och driver allt från smartphones till elbilar. När vi går mot en mer hållbar framtid växer efterfrågan på avancerade batterier snabbt. Föreställ dig batterier som är flexibla och böjbara, kapabla att driva bärbara enheter som övervakar vår hälsa i realtid; batterier som kan driva bilar långa sträckor utan behov av frekventa laddningar; och batterier som är prisvärda och gör elfordon tillgängliga för alla. Dessa krav driver utvecklingen av nya batterier såsom flexibla helorganiska batterier, all-solid-state batterier (ASSB) och natriumjonbatterier (SIB).

Innan dessa nya batteriteknologier når marknaden är det avgörande att förstå deras miljöpåverkan, vilket är fokus för denna avhandling. Detta arbete utforskar miljöprestandan hos ett flexibelt helorganiskt batteri, två ASSB och tre SIB, och jämför dem med traditionella litiumjonbatterier (LIB) genom livscykelanalys (LCA) och prospektiv LCA.

Det helorganiska batteriet visade sig ha högre miljöpåverkan än LIB, eftersom det lagrar mindre energi per massa. Detta innebär att fler batterier krävs för att utföra samma arbete, vilket leder till högre utsläpp under produktionen. Framför allt bidrar katodmaterialen till dessa effekter på grund av deras resursintensiva produktionsprocesser. ASSB visade jämförbar eller högre klimatpåverkan än LIB, främst på grund av de höga utsläppen i samband med produktionen av fasta elektrolyter och katodaktiva material. Klimatpåverkan av SIB varierar, där den skiktade oxidtypen visar en liknande klimatpåverkan som LIB, medan de andra typerna, poly-anjon och preussian blue analog visar högre klimatpåverkan än LIB. Katoden är den största bidragsgivaren för alla tre typer av SIB.

Det är viktigt att notera att dessa jämförelser endast fokuserar på produktionsprocessen. När man beaktar batteriets användningsfas och dess slutskede kan resultaten förändras.

Trots dessa utmaningar kan det fortfarande vara önskvärt att ha dessa avancerade batterier på marknaden på grund av deras funktionella fördelar. Hur kan vi då förbättra deras miljöprestanda? Studierna tyder på att genom att optimera batteridesign, använda mer förnybar elektricitet i tillverkningsprocesser och använda mer återvunnet material kan vi avsevärt minska deras miljöavtryck.

Forskningen i denna avhandling ger värdefulla insikter för batteriutvecklare och hjälper dem att skapa mer miljövänliga batterier som stödjer vår övergång till en hållbar framtid.

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Life cycle assessment of an all-organic battery: Hotspots and opportunities for improvement

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ABSTRACT

Organic batteries are emerging as a potential sustainable power source for future flexible devices. Using life cycle assessment, this study analyzed the environmental impacts from the synthesis process for an all-organic battery with conducting redox polymers as active materials for electrodes. Synthesis steps were modeled and analyzed in detail, based on actual laboratory processes data for electrodes, and industrial data for other battery components. Complete and transparent inventory data are presented and can be used in future environmental assessments. The organic battery studied is still at an early development stage, so environmental hotspots and potential improvements in the synthesis processes were examined. For selected environmental impact categories, the life cycle assessment results showed that synthesis of cathode backbone was the major contributor (47–63%) to the environmental impacts of the all-organic battery cell among different synthesis stages, because of a long synthesis route associated with high solvent usage. Solvents (*e.g.*, dichloromethane), catalysts (*e.g.*, copper oxide, Pd (PPh_3)$_4$), zinc, and waste treatment processes were important single contributors to the total impacts. The results reveal significant potential for improvement by optimizing the amount of solvents needed to synthesize battery electrodes. Changing treatment methods for laboratory waste solvents can also strongly influence the results.

1. Introduction

Flexible and bendable electronics have undergone rapid development over the past few decades, and are now attracting significant attention from the public and researchers (Delaporte et al., 2020; Lee et al., 2018). In the field of medicine and healthcare, flexible electronics are used extensively as wearable devices to track human activity (*e.g.*, steps, calories burned, sleeping hours) and monitor health conditions (Cima, 2014; Miyamoto et al., 2017; Son et al., 2014). In logistics, intelligent packaging with integrated flexible electronics can provide real-time information on the temperature, humidity, location, and quality of products, allowing optimization of transport, improved product quality, and reduced economic losses (de Abreu et al., 2012; Schaefer and Cheung, 2018; Yam et al., 2005). Flexible and bendable electronics are also expected to be applied in displays such as e-books and e-papers, to meet market and customer requirements (Chung and Kang, 2009). Additionally, application of flexible electronics is contributing to the development of soft robot technologies (Rus and Tolley, 2015). These applications could add much convenience to modern life, enabling a further shift from an individual computing paradigm to a hyper-connected society (Choi, 2014). However, to succeed fully in development of flexible electronics, a more flexible and sustainable power supply unit is needed.

Flexible lithium ion batteries are considered a promising energy storage solution for future flexible devices, as they are thin, lightweight, and have high power output and high energy density (Delaporte et al., 2020; Hu et al., 2010; Nyholm et al., 2011). However, issues relating to the use of relatively scarce lithium and cobalt, immature lithium recycling technology, geopolitical and socio-political problems associated with cobalt mining, and the toxicity of cobalt are major concerns (Janoschka et al., 2012; Larcher and Tarascon, 2015; Muench et al., 2016). Zinc ion batteries, and biodegradable transient batteries are other promising flexible battery technologies that is drawing many researchers' attention (Delaporte et al., 2020; Huang et al., 2019; Zhang et al., 2019). However, human toxicity and other environmental issues (*e.g.*, water, soil, plant pollution) caused by metals used for electrodes and current collector (*e.g.*, Zn, Cu) need to be taken into consideration (Mittal et al., 2021). For example, released sulfate and mobile metals

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during zinc mining activities can affect human health and the environment directly and indirectly (Mittal et al., 2021; Zhang et al., 2012).

Compared with these battery materials, organic battery materials can be derived from renewable, non-scarce abundant substances extracted from biomass, avoiding mineral resource depletion. Toxicity effects caused by chemicals used in or generated from traditional batteries production are avoided in organic battery, for example, lead, PF_6^-, and HF (Duehnen et al., 2020; Larcher and Tarascon, 2015). End-of-life disposal will also be facilitated by absence of metals, as the battery can be recycled or incinerated using the same waste treatment route as the product it powers. Organic battery materials are also highly versatile, with a tunable structure and bendable characteristics, making them a very promising next-generation flexible energy power source (Song and Zhou, 2013). However, all-organic batteries are less common. Besides, most organic electrode materials do not supply sufficient conductivity, so a large amount of conductive additives and binders are required in the electrodes of organic battery to increase conductivity and sustain material cohesion (Perticarari et al., 2018, 2019; Tong et al., 2019), which complicates the electrode synthesis process and reduced the energy density of the batteries (Emanuelsson et al., 2017). The organic battery cell assessed in this study is based on a newly developed all-organic battery technology using no additives and binders (Strietzel et al., 2020). Hence, it is considered as a promising all-organic battery with low weight, good stability, and fast charging characteristics with potential to be used in flexible devices.

As technology develops, it becomes more costly and difficult to modify material and production process choices when more knowledge and data become available. This means that decisions made at early stages in development of a technology will have far-reaching influences on its environmental performance in technological applications (Arvidsson et al., 2018; Villares et al., 2017). The importance of evaluating the environmental impacts of technologies at an early stage has been widely acknowledged (Hetherington et al., 2014; Sandin et al., 2014). Given the high potential market prospects of all-organic batteries, there is a need to assess the environmental impacts at an early development stage to prevent future unintentional environmental consequences. Life cycle assessment (LCA) is considered a suitable holistic tool for quantifying cumulative environmental loads of products, processes, or activities throughout their life cycle (Hauschild, 2005; Hellweg and Canals, 2014). LCA can cover all stages of a product's life cycle, from raw material extraction to end-of-life disposal or recycling, and can take various environmental impact categories into consideration. This can prevent environmental burden shifting between life cycle stages and environmental impact categories (Kleinekorte et al., 2020). To our knowledge, this is the first LCA study of all-organic batteries. The overall aim of the present study was to provide environmental guidance on future development of an organic battery cell. Specific objectives were (1) to investigate the environmental performance of the all-organic battery described by Strietzel et al. (2020); (2) to identify environmental hotspots in the life cycle stages of this battery; and (3) to identify opportunities to reduce the environmental impacts at an early stage of the development.

2. Materials and method

A cradle-to-factory gate LCA was conducted to quantify the environmental impacts of all synthesis processes of the all-organic battery cell at laboratory-scale. The LCA was conducted in accordance with ISO 14040/44 international standards and the ILCD handbook (Hauschild et al., 2011; ISO, 2006a, 2006b), comprising the four standard phases: goal and scope definition, life cycle inventory (LCI), life cycle impact assessment (LCIA), and interpretation.

2.1. Goal and scope

The goal was to perform a detailed life cycle inventory and assessment of the laboratory-scale synthesis system for an organic battery, to provide environmental guidance in its early-stage development. The functional unit (FU) was one 3 cm by 3 cm organic battery cell prototype. The estimated technology readiness level and manufacturing readiness level are around four. The results were not compared with those of other LCA studies on battery cells, because the organic battery is an emerging technology with unique applications and there is no product with similar applications currently on the market. Hauschild et al. (2018) state that a comparison in LCA is only valid when the products compared provide the same functions. Comparing laboratory-scale processes with industrial-scale processes is another recognized challenge (Hetherington et al., 2014; Pallas et al., 2020; van der Giesen et al., 2020). The environmental impacts calculated from laboratory data are usually much higher than those calculated from industrial data on a mature system (Gavankar et al., 2015). The second functional unit 1 kWh stored electricity is used to facilitate comparison for later lab-scale organic battery studies. Since it is not the aim of the study, the results will not be discussed in this paper, but can be found in Table S3.5. Battery usage and end-of-life treatment stages were not considered in this study. Fig. 1 presents the system boundary of the study, which covered three groups of processes (upstream, laboratory, and downstream):

1. Upstream processes include raw materials extraction, transportation, battery chemicals manufacturing, and precursor chemicals manufacturing. Raw material extraction refers to acquisition of natural resources for manufacturing chemicals that can be used directly or indirectly in the organic battery cell components. Battery chemicals manufacturing refers to production of chemicals that can be used directly as battery components, *e.g.*, electrolyte, current collector, separator, and battery casing. Precursor chemicals manufacturing refers to production of chemicals needed for synthesizing battery electrodes.
2. Laboratory processes include synthesis of anode and cathode and assembly of the battery. The laboratory synthesis routes are depicted in Fig. 2.
3. Downstream processes manage different types of waste flows from upstream processes and laboratory processes.

2.2. Life cycle inventory (LCI) and data sources

The all-organic battery cell assessed in this study was developed by the Nanotechnology and Functional Materials group at Uppsala University (Strietzel et al., 2020), which provided laboratory process data for the present analysis. Data on upstream processes (Section S1 in Supplementary Material) were obtained from the Ecoinvent 3.6 database (cut-off) whenever possible (processes in grey in Fig. 2). Data not available in the database were generated by determining the production routes, based on information from patents and the literature (processes in orange in Fig. 2). Among the data used for downstream processes, parameters for waste solvent distillation processes were taken from Capello et al. (2005) (Table S3.1). Data on waste treatment processes from the Ecoinvent 3.6 database (cut-off) were also used. In the LCI phase of the assessment, the data were complemented with ancillary inputs calculated by parameters from the literature (Capello et al., 2005; Geisler et al., 2004; Piccinno et al., 2016), *e.g.*, energy requirement, cooling water, *etc.* A data inventory for each chemical produced from upstream processes can be found in Tables S1.1-21 in Supplementary Material.

2.2.1. Battery technology and synthesis stages

The battery cell assessed has a mass of 483.23 mg, an active area of 9 cm^2 (3 cm × 3 cm), and a casing area of 12.25 cm^2. The specific capacity is 60 mAh/g of electrode active material, the capacity is 1.08 mAh, the voltage is 0.4 V, and the specific energy is 0.9 Wh/kg. According to Strietzel et al. (2020), the battery can retain 85% of initial capacity after

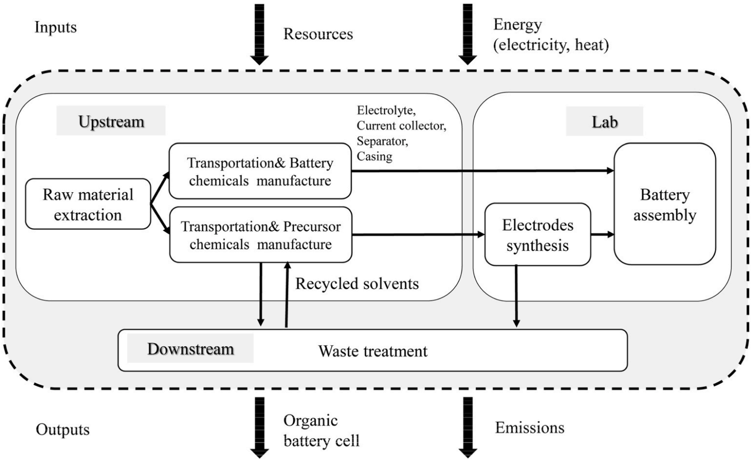

Fig. 1. System boundary (dashed line) of the present study and the three groups of processes covered in the analysis (upstream, laboratory, downstream).

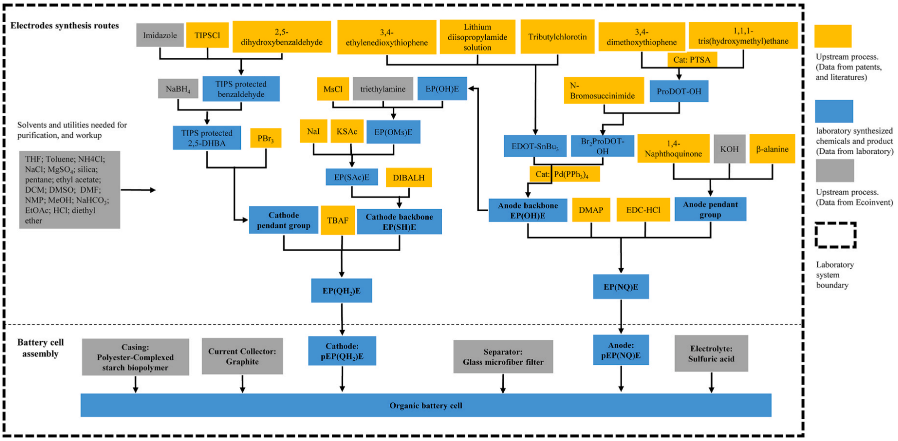

Fig. 2. Laboratory synthesis routes for an organic battery cell. The dashed line divides the laboratory synthesis into electrodes synthesis routes and battery cell assembly. Chemical structures for ProDOT-OH, Br_2ProDOT-OH, EDOT-SnBu3, and TIPS protected 2,5-DHBA can be found in Fig. S2 in Supplementary Material. TIPSCl = Triisopropylsilyl chloride, PTSA = Para-toluenesulfonic acid, MsCl = Methanesulfonyl chloride, KSAc = Potassium thioacetate, DIBALH = Diisobutylaluminum hydride solution, TBAF = Tetra-n-butylammonium fluoride, DMAP = 4-dimethylaminopyridine, EDC-HCl = N-(3-dimethylaminopropyl)-N′-ethylcarbodiimide hydrochloride.

500 charge-discharge cycles, can be fully charged within 100 s, and can maintain good performance at low temperatures, even down to −24 °C.

The battery cell consists of six components: cathode, anode, electrolyte, current collector, separator, and battery cell casing. Table 1 sums up the inventory of one organic battery cell. The electrodes (anode and cathode) consist of two conducting redox polymers (CRPs) as active materials. These two CRPs are composed of polymeric backbones, with trimeric repeat units, and two different pendant groups (naphthoquinone and hydroquinone, respectively). The trimers (EPE) were formed by attaching two 3,4-ethylenedioxythiophene (EDOT, E) at central 3,4-propylenedioxythiophene (ProDOT, P)'s α-positions (Fig. S2, Synthesis of anode backbone). When polymerized polymer backbone serves as to provide electronic conductivity and reduce the solubility of CRPs in the electrolyte. The pendant groups are benzoquinone/hydroquinone (Q/QH_2) and naphthoquinone/naphthohydroquinone (NQ/NQH_2) for cathode and anode, respectively. Pendant groups are capacity carriers in the two electron/two proton ($2e^-/2H^+$) quinone/hydroquinone redox reaction during the organic battery's charge/discharge activity. QH_2 and NQ moieties are attached to the central unity of the trimeric EPE structure, to synthesize the monomers EP(QH_2)E, and EP(NQ)E (Fig. S2). These two monomers are subsequently polymerized to form the CRPs pEP(QH_2)E, and pEP(NQ)E, as the cathode and anode active materials, respectively.

Of the other four battery components, the electrolyte is sulfuric acid (0.5 M), which provides protons, allowing the QH_2 and NQ $2e^-/2H^+$ redox reaction to occur. A glass microfiber filter is used as the separator.

Table 1
Inventory overview for one 3 cm by 3 cm size organic battery cell.

Battery component	Active material	Mass, mg	Inventory process
Cathode	pEP(QH_2)E[a]	18	Own process, based on actual synthesis
Anode	pEP(NQ)E[a]	18	Own process, based on actual synthesis
Current collector	Graphite	9	Market for graphite, battery-grade (global data from Ecoinvent 3.6)
Separator	Glass microfiber filter	46.23	Market for glass fiber (global data from Ecoinvent 3.6)
Electrolyte	0.5 M H_2SO_4	24.5	Market for sulfuric acid (European data from Ecoinvent 3.6)
Battery casing	Biopolymer plastic	367.5	Market for polyester-complexed starch biopolymer (global data from Ecoinvent 3.6)

[a] In pEP(QH_2)E and pEP(NQ)E, E refers to 3,4-ethylenedioxythiophene; NQ refers to naphthoquinone; P refers to 3,4-propylenedioxythiophene; p refers to polymerized; Q refers to benzoquinone; QH_2 refers to hydroquinone.

The current collector is made from Asahi TU-10S carbon conductive paste but, due to lack of data, pure graphite was modeled here as an alternative as Asahi TU-10S carbon paste contains carbon nanoparticles with large amount of graphite particles. The battery cell package is made from plastic (Dupont FEP 500C film), but polyester-complexed starch biopolymer material was used in modeling due to data limitations.

Based on electrode chemical structure (backbone and pendant group), the all-organic battery synthesis routes can be divided into seven synthesis stages: synthesis of anode backbone, synthesis of anode pendant group, synthesis of anode, synthesis of cathode backbone, synthesis of cathode pendant group, synthesis of cathode, and non-electrode components production (Fig. 3). Each synthesis stage includes one or more chemical synthesis processes, as Fig. 3 shows. ProDOT-OH, Br_2ProDOT-OH, EDOT-SnBu_3, and EP(OH)E are used in both anode and cathode synthesis. A detailed description of synthesis stages and relevant inputs and outputs flows can be found in Section S2 in Supplementary Material.

2.2.2. Assumptions

The following general assumptions were made in the LCI:

1) Swedish and European data from the Ecoinvent 3.6 database were used, when available. Otherwise, global data were used.
2) The reaction yield for chemical products was 95% if process-specific information was missing (Wernet et al., 2012).
3) Electricity at medium voltage from Sweden was used as the electricity source.
4) 100% of the electricity and heat from steam consumed was converted to waste heat, and no heat recovery was assumed.
5) The cooling water was not contaminated during the process, and 100% of the cooling water was returned untreated to the biosphere after use.
6) Metallic catalysts used in industry are likely to be recycled due to their economic value, but catalysts are usually ignored in LCA studies (Parvatker and Eckelman, 2019), which might lead to major uncertainties in the results. Following the suggestion in Piccinno et al. (2016), it was assumed that no catalyst was recycled and a sensitivity analysis was performed to evaluate how this assumption affected the final results.
7) All processes are balanced in terms of inputs and outputs.
8) Waste solvents generated from upstream processes were recycled using distillation, and modeled according to parameters from Capello et al. (2005) (Table S3.1). Waste solvents generated in the laboratory process were treated using the “spent solvent mixture” process from Ecoinvent 3.6 database.

It is worth noting that the above eight assumptions only applied to the processes that we built ourselves. Specifically, assumptions 1, 3, 4, 5, 7 applied to all processes, while assumption 8 only applied to downstream processes and assumptions 2 and 6 only applied to upstream processes.

2.2.3. Energy requirement

When data on energy requirement were not available, energy requirement was calculated according to Piccinno et al. (2016) (Equation (1), (3), (4)), and Arvidsson et al. (2014) (Equation (2)). In this study, energy requirement only included the supplied heat (Q_{supply}), and the electricity for stirring (E_{stir}). The supplied heat (Q_{supply}) can be calculated as the sum of energy needed to reach the reaction temperature (Q_{heat}) and the heat loss (Q_{loss}), divided by the efficiency of the heating device (η_{heat}) (Equation (1)).

$$Q_{supply} = \frac{Q_{heat} + Q_{loss}}{\eta_{heat}} \tag{1}$$

The energy needed to reach the reaction temperature Q_{heat} can be calculated from Equation (2).

$$Q_{heat} = C_p * m_{mix} * \Delta T \tag{2}$$

where C_p is specific heat capacity of the main solvent (in J/g*K), m_{mix} is the mass of the reaction mixture (including solvent and reactants), and ΔT is the temperature difference between starting temperature and reaction temperature. If solvent mixtures are used, the specific capacity is estimated using a mole fraction average of each solvent component. Here, it was assumed that reagents were dissolved in solvents for all chemical reactions. To simplify the calculations, the influence of the reagents on the specific capacity of the mixture was neglected.

The energy needed to compensate for the heat loss Q_{loss} is the energy loss from the reactor surface, which can be calculated using equation (3).

$$Q_{loss} = A * \frac{k_a}{s} * \Delta T * t \tag{3}$$

where A is the surface area of the reactor, k_a is the thermal conductivity of the insulation material, s is the thickness of the insulation, ΔT is the temperature difference between the inside and outside of the reactor (ΔT), and t is the reaction temperature. For the reactor-related parameters (A, k_a, s), average data from Piccinno et al. (2016) were used in this study.

Stirring energy can be calculated using equation (4):

$$E_{stir} = \frac{N_p * \rho_{mix} * N^3 * d^5 * t}{\eta_{stir}} \tag{4}$$

where N_p is power number of the impeller, ρ_{mix} is density of the reaction mixture, N is rotational speed of the agitator, d is diameter of the impeller, t is reaction time, and η_{stir} is efficiency of the agitator. For the impeller-related parameters (N_p, ρ_{mix}, N, d, η_{stir}), average data from Piccinno et al. (2016) were used in this study.

2.3. Life cycle impact assessment (LCIA)

The International Reference Life Cycle Data System (ILCD) 2011 midpoint method was used to calculate the environmental impact category indicators. The ILCD method, which was developed by the European Commission - Joint Research Center (EC-JRC), includes 16 recommended impact categories, associated LCIA models, and characterization factors. These recommended LCIA models and characterization factors were selected from existing LCIA methods according to certain criteria for each impact category. (Hauschild et al., 2011). The inventory and the impact calculations were modeled in SimaPro® software.

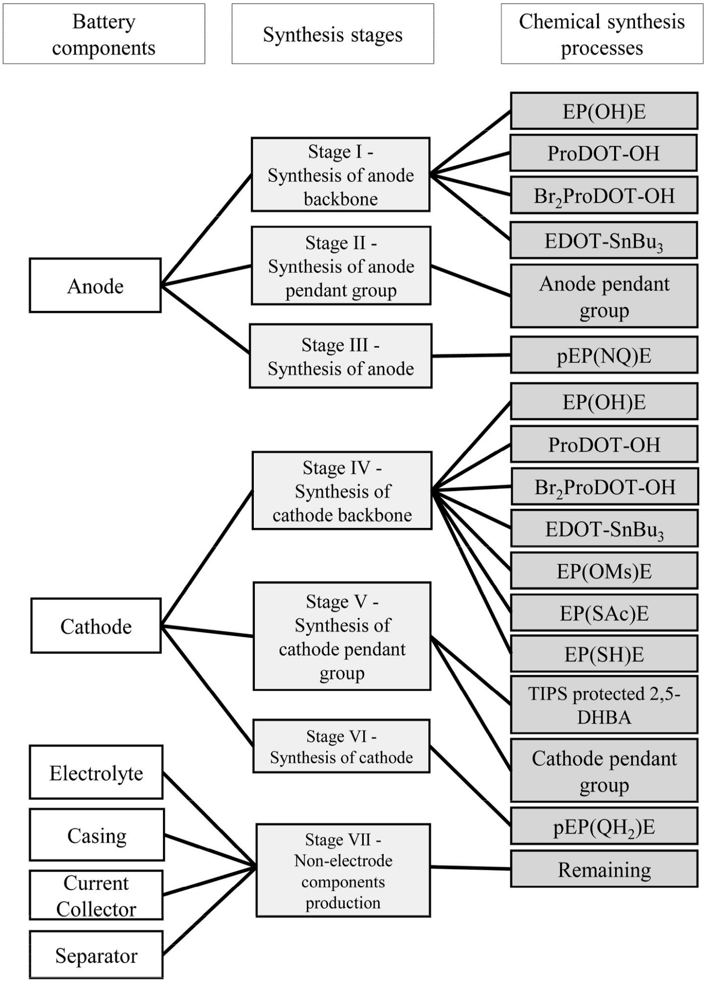

Fig. 3. The chemical synthesis processes are categorized in seven synthesis stages for the assembly of the six components of the all-organic battery cell.

The units of the characterization results vary for each impact category, making it unfeasible to compare them. Normalization and weighting can be applied to determine the most important impact categories for the studied system and for each synthesis stage. The purpose of normalization is to present the relative magnitude of each characterized score by relating it to a common reference system, using normalization factors (Hauschild et al., 2018). The EC-JRC Global normalization factors, which indicate the global impacts per person for each impact category in the reference year 2010 (Benini et al., 2015), were used in this study. For each impact category c, the normalized score (NS_c) was calculated by dividing the impact score (IS_c) by the corresponding normalization factor (NF_c) (Equation (5)):

$$NS_c = IS_c / NF_c \tag{5}$$

In this study, a normalization factor (NF) was calculated for each impact category (c) by dividing the total global impacts of each impact category by the global population (P_g), according to equation (6). The total global impact for each impact category is then the sum of impacts of all elementary flows included in the impact category.

$$NF_c = \frac{\sum_i (CF_i * E_i)}{P_g} \tag{6}$$

where subscript *i* indicates each elementary flow included in an impact category, CF_i is the characterization factor of elementary flow *i*, and E_i is the amount of elementary flow *i* that is released to or extracted from the environment in the reference year 2010 (Hauschild et al., 2018).

Weighting can only be applied based on normalization scores. It supports identification and prioritization of the most relevant impacts categories by applying different weights to each impact indicator (Hauschild et al., 2018). The ILCD weighting factors used in this study include public and LCA expert opinions and the level of impact for each impact category compared to the planetary boundaries (Serenella et al., 2018). Weighted results for each impact category were calculated by multiplying normalized scores of each impact category by the corresponding weighting factors.

The most relevant impact categories for organic battery cell production systems were calculated by following the Product Environmental Footprint Category Rules Guidance (PEFCR), which suggests that the most relevant impact categories should be selected according to the normalized and weighted LCA results, and should be identified as impact categories with a cumulative contribution of more than 80% of the total environmental impacts, without considering toxicity-related impact categories (European Commission, 2018). Following this guidance, four impact categories were considered to be most important in this study: mineral, fossil, and renewable resource depletion (in kg antimony (Sb) eq); climate change (in kg CO_2 eq); ozone depletion (in kg CFC-11 eq); and particulate matter (in kg PM2.5 eq) (Table S3.3 in Supplementary Material).

There is a debate on whether current toxicity-related impact categories are robust enough to be included in LCA (European Commission, 2018; Heijungs et al., 2007; Luca et al., 2016; Vincent-Sweet et al., 2017). This is mainly due to limited elementary flows included in calculation of characterization factors, high uncertainties in modeling fate and exposure, unclear definition of the toxic effects, and unclear mechanisms of the action of metals (Benini et al., 2014; Pizzol et al., 2011). Despite these uncertainties, it is not uncommon for LCA studies to include toxicity-related impact categories in hotspot analysis, to provide more complete results (Gear et al., 2018; Isola et al., 2017; Liu et al., 2015; Troy et al., 2016; Vincent-Sweet et al., 2017). In conventional battery production, metals (*e.g.*, lead (Pb), nickel (Ni), Cu, Al) are usually the main contributors to human or ecological toxicity potential (Ellingsen et al., 2014; Liu et al., 2015; Majeau-Bettez et al., 2011; Wang et al., 2018). No metals are directly used as components in the organic battery cell analyzed in the present study, but some metals are involved in the upstream processes. Therefore, toxicity impacts were included in order to assess whether metals used in the upstream processes, and other chemicals used in the system, contribute significantly to the environmental impacts. Three toxicity-related impact categories were included in the study according to the normalized and weighted results: freshwater ecotoxicity, human toxicity with cancer effects, and human toxicity with non-cancer effects (Table S3.3).

3. Results and discussion

3.1. *Midpoint impact results*

Results for selected impact categories are summarized in Table 2. All results for ILCD 2011 midpoint categories can be found in Table S3.4-3.5 in Supplementary Material. Overall, electrode (anode and cathodes) synthesis accounted for approximately 99.5–99.9% of the environmental impact for all selected categories, even though electrodes only account for 7% of the total battery cell mass. This is because the inventory data used for electrodes were based on laboratory-scale data, while other battery components were modeled using industrial-scale data. It is worth noting that the mass of electrodes usually account for more than 50% of the total battery cell weight (Deng et al., 2017a; Peters et al., 2016). The low mass proportion of electrodes in the all-organic battery cell is caused by the low technology readiness level of the battery cell and the small scale fabrication technology (laboratory-level). An increase in electrodes' mass percentage can be expected in the future. Previous studies have shown that the environmental impacts of a product decrease with increasing production scale and increasing technological maturity (Gavankar et al., 2015; Troy et al., 2016). Comparing the two different electrodes, the cathode showed higher environmental impacts than the anode for all environmental impact categories, with synthesis stage of cathode backbone being the greatest contributor (Table 2). This was due to the many synthesis steps required in the synthesis stage of cathode backbone, resulting in high consumption of chemicals needed for work-up and purification (*e.g.*, solvents, silicon, Na_2SO_4, etc.) and a larger amount of waste generated.

Fig. 4 summarizes the main contributors for different impact categories. For mineral, fossil, and renewable resource depletion, zinc and catalysts were the greatest contributors. Zinc, a reagent used for producing EDOT (the precursor for the electrode backbone) emerged as the major single contributor, accounting for 52% of the total impact. Production of $Pd(PPh_3)_4$, which is used as a catalyst for synthesizing electrode backbone EP(OH)E, was also responsible for a major share (40%) of the total resource depletion. Therefore, in total more than 90% of the resource depletion was accounted for by anode and cathode backbone synthesis.

For other impact categories, solvent use was clearly the greatest contributor, accounting for 37–100% of the total impact (Fig. 4). Dichloromethane (DCM), ethyl acetate, pentane, tricholoromethane, and tetrahydrofuran (THF) are used as eluents in flash column chromatography for purification and as media for chemical reactions. In general, synthesis stages with purification processes showed higher impact potential, *i.e.*, Synthesis stages of anode backbone, anode, cathode backbone and cathode (Table 2). Synthesis of cathode backbone showed the highest impact of all seven synthesis stages (Table 2), due to the four chemical reactions in cathode backbone synthesis (synthesis process EP(OH)E, ProDOT-OH, EP(OMs)E, and EP(SAc)E) requiring purification processes (Fig. 3). The environmental impacts caused by

Table 2

Life cycle assessment (LCA) characterization results based on one 3 cm by 3 cm organic battery cell as the functional unit (FU), and percentage of the total environmental contribution from different battery components and synthesis stages. * Stage I= Synthesis of anode backbone, Stage II= Synthesis of anode pendant group, Stage III= Synthesis of anode, Stage IV= Synthesis of cathode backbone, Stage V= Synthesis of cathode pendant group, Stage VI= Synthesis of cathode, Stage VII = Non-electrode components production.

Impact category	Value (per FU)	Percentage by synthesis stages						
		Anode			Cathode			Remaining battery components
		Stage I*	Stage II*	Stage III*	Stage IV*	Stage V*	Stage VI*	Stage VII*
Climate change	3.3 x 10^{-1} kg CO_2 eq	12%	2%	19%	47%	5%	15%	0%
Ozone depletion	1.9 x 10^{-6} kg CFC-11 eq	7%	3%	1%	62%	4%	22%	0%
Human toxicity, non-cancer effects	6.7 x 10^{-8} CTUh	19%	2%	15%	51%	4%	9%	0%
Human toxicity, cancer effects	1.3 x 10^{-8} CTUh	14%	5%	16%	47%	5%	13%	0%
Particulate matter (PM)	2.3 x 10^{-4} kg PM2.5 eq	9%	2%	13%	52%	5%	19%	0%
Freshwater ecotoxicity	4 CTUe	22%	1%	17%	50%	4%	6%	0%
Mineral, fossil & renewable resource depletion	3.8 x 10^{-5} kg Sb eq	34%	0%	2%	63%	1%	1%	0%

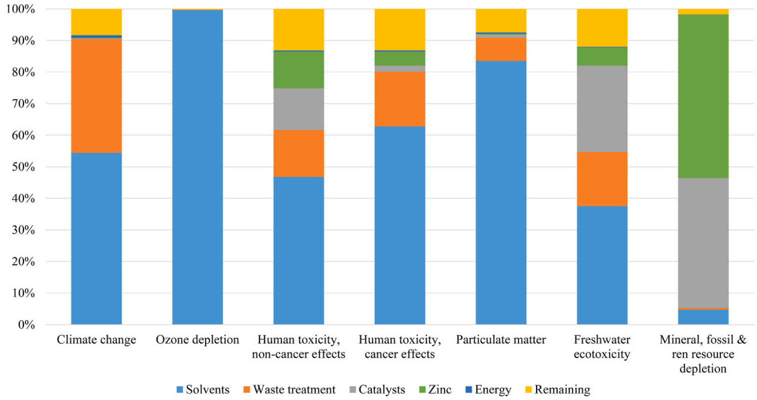

Fig. 4. Contribution of different process flows in synthesis of one 3 cm by 3 cm organic battery cell to selected impact categories. ren. = renewable.

different solvents differ. For example, this study showed that, for the same amount of THF, DCM, and pentane, the climate change caused by THF is the greatest, followed by DCM and pentane. Similar results have been found in a previous study (Amelio et al., 2014).

The ozone depletion category was affected most by use of solvents (Fig. 4). About 99% of the ozone depletion potential was due to use of DCM (82%) and trichloromethane (17%). Dichloromethane is widely used in synthesis stage of cathode backbone for synthesis of intermediate chemical EP(OMs)E, EP(SAc)E, and EP(SH)E, and in synthesis stage of cathode. The increased emissions with use of DCM could affect the rate of stratospheric ozone recovery (Hossaini et al., 2015; Liang et al., 2017). Trichloromethane is used as a solvent in upstream processes, for synthesizing intermediate chemicals ProDOT-OH and EDOT-$SnBu_3$ in anode and cathode backbone synthesis stages, respectively. Pallas et al. (2020) identified trichloromethane as a major contributor to ozone depletion in a solar cell production system. The by-product of trichloromethane production, tetrachloromethane (CCl_4), is also a long-lived ozone-depleting substance (Liang et al., 2017).

The materials used for assembling the all-organic battery cell was clearly lacking toxic materials such as $LiPF_6$, which is used in traditional batteries (Duehnen et al., 2020). However, the solvents and indirectly used metals also contributes to the environmental impact. The result shows that use of solvents was the dominant contributor to freshwater ecotoxicity (37%) and human toxicity with cancer (63%) and non-cancer effects (47%) in the present analysis (Fig. 4). According to Heppel et al. (2011), DCM can be absorbed, distributed, and disseminated rapidly in the human body. Animal tests show that DCM can also cause cancer (Tsai, 2017). Copper oxide (CuO), which is used as a catalyst for producing the precursor (EDOT) of the electrode backbone EP(OH)E, was another major toxicity source, representing 13% and 27% of the impacts for human toxicity with non-cancer effects and freshwater ecotoxicity, respectively. Copper, used as the current collector in other batteries, is often reported to be the main contributor to toxicity-related impact categories (Deng et al., 2017b; Ellingsen et al., 2014; Wang et al., 2020). Again, as it has been discussed before, toxicity related impact categories have higher uncertainty comparing with other environmental impacts.

Waste treatment contributed to climate change (36%), human toxicity with cancer (17%) and non-cancer effects (15%), freshwater ecotoxicity (17%), and particulate matter (7%). There was also a positive correlation between the amount of waste and the amount of solvent used, *i.e.* the amount of waste to be handled increased with increasing solvent use.

3.2. *Energy requirement*

Synthesis of one 3 cm by 3 cm organic battery required 20.2 kJ of heat (generated from steam), and 7.4 kJ of electricity. Heat was used for waste solvent distillation in upstream and downstream processes, and electricity used for cooling or heating chemical reactions, and for waste solvent distillation. Most of the energy requirement was attributable to upstream and downstream processes, including 100% of the heat and 60% of the electricity (Fig. 5). Owing to the relatively low reaction temperatures needed for the chemical reaction steps (usually room temperature), less electricity was required in the laboratory synthesis processes. Due to lack of data, energy requirement was estimated in this study using mathematical equations from small industrial-scale production, which is a source of uncertainty. Therefore, energy requirement in the laboratory synthesis processes might have been underestimated. However, the extremely small overall contribution of energy requirement to different impact categories (Fig. 4) indicates that improving the energy efficiency in future optimization will not contribute substantially to improving the environmental impact.

3.3. *Normalized and weighted results*

The normalized and weighted environmental impacts contributed by each production stage for one 3 cm by 3 cm organic battery are shown in Fig. 6. In most of the synthesis stages, human toxicity with cancer effects was the category making the greatest contribution (21–50% of total impact), except in synthesis stage of anode backbone, and non-electrode components production stage. Freshwater ecotoxicity (10–34%) was another important contributor in most synthesis stages. Resource depletion contributed most in synthesis stage of anode backbone (30%), and was also a dominant contributor to environmental impact in synthesis stage of cathode backbone (19%). Ozone depletion made important contributions in synthesis stage of anode pendant group, cathode backbone, cathode pendant group, and synthesis stage of cathode. In general, climate change, human toxicity with non-cancer effects, and particulate matter had rather low normalized and weighted environmental impacts.

3.4. *Sensitivity analysis*

A number of parameters used in the model have high uncertainty, which means that the parameter value may change and the value used in the model might not always represent reality. To determine how the results were affected by different parameters, a sensitivity analysis was

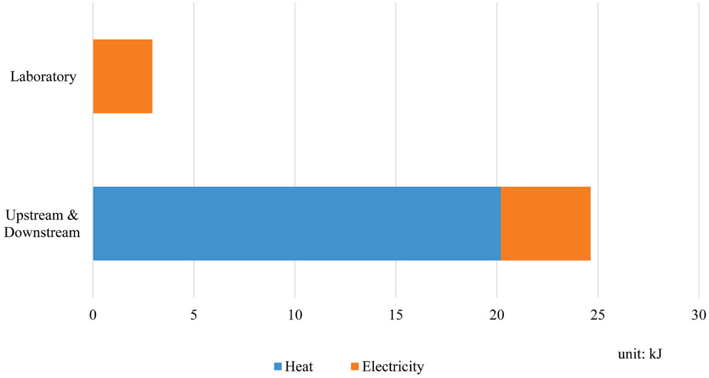

Fig. 5. Energy requirement for synthesizing one 3 cm by 3 cm organic battery cell.

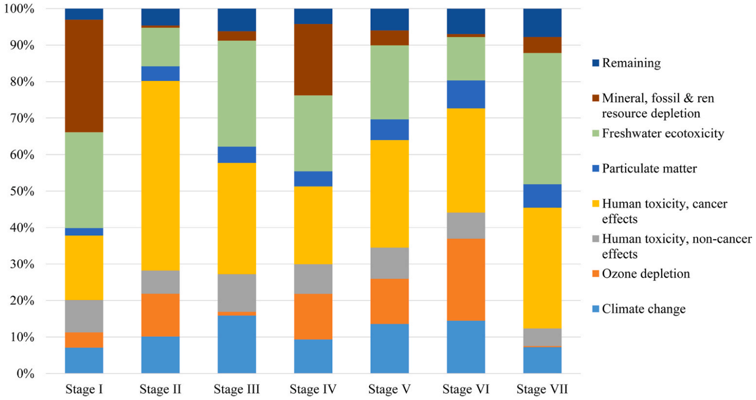

Fig. 6. Normalized and weighted environmental impacts contributed by each production stage (I-VII) in synthesis of one 3 cm by 3 cm organic battery cell. ren. = renewable. * Stage I= Synthesis of anode backbone, Stage II= Synthesis of anode pendant group, Stage III= Synthesis of anode, Stage IV= Synthesis of cathode backbone, Stage V= Synthesis of cathode pendant group, Stage VI= Synthesis of cathode, Stage VII = Non-electrode components production.

performed. The parameters tested in the sensitivity analysis were a) reaction yield, b) catalyst recovery rate (only for catalysts used in upstream processes), and c) laboratory waste solvent treatment method. Furthermore, three scenarios regarding the amount of solvents used at laboratory processes were applied.

It was assumed that the reaction yield for chemical products was 95% when relevant information was missing. Values of 80%, 85%, and 97% were tested in the sensitivity analysis. The results showed that changes in reaction yield had very little effect on the results (<1%) (Table S3.6 in Supplementary Material).

Two catalysts used in the upstream processes are copper oxide and tin(II) chloride ($SnCl_2$). Tests on catalyst recovery rates of 50%, 90%, 99%, and 100% in the sensitivity analysis revealed minor changes (<1%) for all impact categories except freshwater ecotoxicity and human toxicity with non-cancer effects (Table S3.7 in Supplementary Material). The freshwater ecotoxicity impacts decreased by up to 32% and the human toxicity with non-cancer effects decreased by up to 11% when the 100% catalyst recovery rate was applied, due to copper oxide being the main contributor to these two impact categories.

All waste solvents generated in the laboratory processes were assumed to be treated as in the method “spent solvent mixture” from Ecoinvent 3.6 in the baseline scenario. In “Spent solvent mixture” treatment method, around 62% of the solvent were treated with incineration, and rest of the solvent were used as a fuel in cement industries (Valsasina, 2011). Other common technologies to deal with waste solvents include incineration and distillation (Kralisch et al., 2015). Therefore, four waste solvent treatment scenarios were tested in the sensitivity analysis: (1) incineration; (2) recycling by distillation with best-case parameters (Table S3.2 in Supplementary Material); (3) recycling by distillation with average parameters (Table S3.2); and (4) recycling by distillation with worst-case parameters (Table S3.2). The results of the sensitivity analysis are shown in Fig. 7. The results for scenarios (2) and (3) indicated that recycling solvents by distillation can potentially reduce the environmental impacts compared with “spent solvent mixture” treatment and incineration.

In laboratory processes involved in synthesis of the organic battery cell, solvents are used in the synthesis of electrodes’ active materials. Solvent usage in the laboratory is currently not optimized, since the focus of technological development is the performance of the final product. Geisler et al. (2004) estimated the minimum (0.2 kg) and maximum (4 kg) amount of solvent needed for producing one kg of chemical product, according to on-site data from a large size plant and

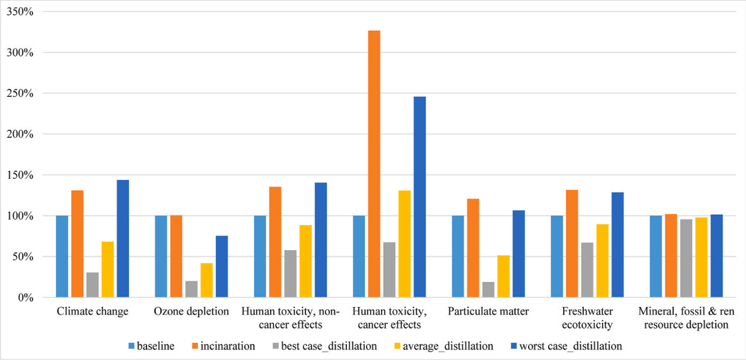

Fig. 7. Influence of different waste solvent treatment methods on the total environmental impact from synthesis of one 3 cm by 3 cm organic battery.

pilot processes, respectively. Piccinno et al. (2016) suggested that a 20% reduction in solvent use is realistic when scaling up from a laboratory process to an industrial process, based on expert opinion. According to the information provided in these two studies, three scenarios were established to assess the influence of excessive solvent use and the potential for improvement:

Scenario 1: 0.2 kg of solvent is used for producing 1 kg of chemical product
Scenario 2: 4 kg of solvent is used for producing 1 kg of chemical product
Scenario 3: A 20% of reduction for laboratory solvent use is applied

The results showed that reduction in environmental impacts under different scenarios vary considerably (Fig. 8). Applying scenario 1 gives the biggest environmental impacts reduction, reducing 5–88% of impacts for all selected impact categories, while applying scenario 3 gives relatively small environmental impacts reduction (Fig. 8). Such difference in results is due to the very high amount of solvents used at laboratory scale, (*e.g.*, usually more than one solvent is used in each chemical synthesis process and single solvent usage can be even up to 80 times of the amount of produced chemical). The rapid reduction of environmental impacts caused by scenario 1 and 2 indicates the big potential in environmental impacts reduction for different environmental impact categories after scaling up the organic battery laboratory system to industrial manufacturing. Additionally, it also indicates the uncertainties of the laboratory-scale LCA, which is in accordance with Pallas et al. (2020), who discussed that improvements on production efficiency should be expected as the emerging technologies scale up from lab to industrial scale.

When scaling up the organic battery laboratory system to industrial manufacturing, improvements in material and energy use efficiency, and the production yield can be expected. The results from three solvent usage scenarios implied that the relative contribution of solvents would most likely be reduced after scaling up to industrial scale production. Consequently, the relative contribution of other process flows will increase and be more visible, like waste treatment processes, energy requirement, nitrogen (used as an inert gas in chemical reactions and solvent recycling processes). Additionally, human toxicity, cancer effects potential, freshwater ecotoxicity potential, and mineral depletion potential can be further reduced if considering catalysts reuse. Even upscaling the laboratory system to industrial production, the electrodes will likely continuously be the dominating contributors among battery components, with the production stage of cathode backbone being the major contributor.

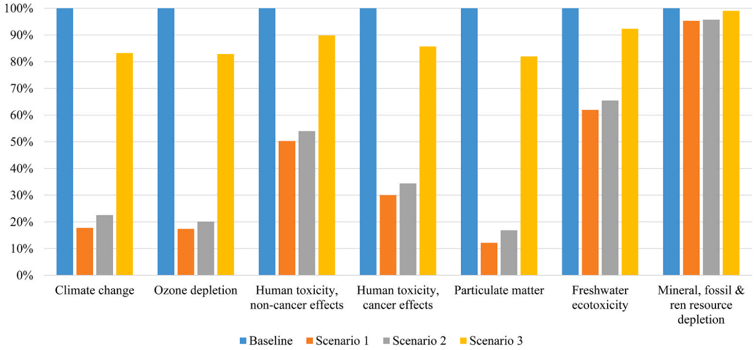

Fig. 8. Influence of amount of solvent use on the environmental impacts from synthesis of one 3 cm by 3 cm organic battery. Scenario 1: 0.2 kg of solvent is used for producing 1 kg of chemical product; Scenario 2: 4 kg of solvent is used for producing 1 kg of chemical product; Scenario 3: A 20% of reduction for laboratory solvent use is applied.

3.5. Opportunities for improvement and future study

Based on the results obtained, solvent use is the hotspot for most environmental impact categories. To reduce the environmental impacts caused by solvent use, the amount of the solvents used in the laboratory needs to be optimized, especially in synthesis stage of anode, cathode and cathode backbone. Recovery of laboratory solvents, *e.g.*, by rotary evaporation, could be another way of reducing environmental impacts, as could using 'green' solvents to replace solvents with high environmental impacts. For example, previous studies recommend use of methanol and acetone to replace DCM, to lower the toxicity (Isola et al., 2017; Montazeri and Eckelman, 2016). According to Cseri. et al. (2018), using solvents like ethyl acetate and toluene is more sustainable than using DCM for the purpose of extraction. Besides, since solvents are used in chemical reactions and purification processes, a shorter synthesis route is an opportunity to reduce the environmental impact from the system, especially for cathode backbone synthesis stage. Production of EDOT (the precursor for the electrode backbone) is also relevant for the overall environmental performance, due to the use of zinc and copper oxide. Reducing the use of EDOT or looking for other alternatives could be a way of reducing the impacts, but would require more detailed research and development. Additionally, looking for other catalysts to replace $Pd(PPh_3)_4$ is a potential way of reducing environmental impacts.

This laboratory-scale LCA provides technology developers with environmental hotspots at the organic battery's early development stage, further guiding the sustainable development of the all-organic battery technology with providing potential opportunities for improvements. Results of this study further contribute to the discussion on the usefulness of lab-scale LCA: laboratory-scale LCA studies should not be used for comparison with established technologies, but to help with the sustainable development of the emerging technologies by identifying the environmental hotspots (Pallas et al., 2020). On the basis of this study, future research on assessing environmental impacts of organic battery at industrial level, with considering the potential improvements of battery performance can be done.

4. Conclusions

This assessment showed that the cathode backbone synthesis stage had the greatest environmental impact (47–63% for different impact categories), due to the long synthesis route and associated large amounts of solvent use and waste. Laboratory solvent use, catalyst use, and waste treatment processes were the main contributing factors to the overall environmental impacts. These results suggest that a shorter synthesis route, optimization of solvent use, recycling of laboratory waste solvents, and reducing or replacing the use of EDOT, and $Pd(PPh_3)_4$ can potentially reduce the overall environmental impacts from synthesis of the organic batteries.

CRediT authorship contribution statement

Shan Zhang: Conceptualization, Methodology, Data curation, Formal analysis, Writing – original draft. **Niclas Ericsson:** Conceptualization, Methodology, Writing - review & editing. **Per-Anders Hansson:** Supervision, Conceptualization. **Martin Sjödin:** Supervision, Investigation. **Åke Nordberg:** Supervision, Conceptualization, Writing - review & editing.

Declaration of competing interest

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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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.jclepro.2022.130454.

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Prospective life cycle assessment of a flexible all-organic battery

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ABSTRACT

Strong interest from researchers and industry is accelerating development of flexible energy storage technologies for future flexible devices. It is critical to consider the environmental perspective in early development of new emerging technologies. In this study, cradle-to-factory gate prospective life cycle assessment (LCA) was performed on production of an all-organic battery with conductive redox polymers as electrode material. To gain a better understanding of the environmental performance of the all-organic battery, a flexible lithium-ion (Li-ion) battery with lithium titanate oxide and lithium cobalt oxide as electrode active materials was modeled as reference. Main environmental impacts of the all-organic battery were attributable to anode and cathode production, with electrode backbones being the main contributors. Solvents, catalysts, waste treatment, energy, and bromine were key individual contributors. Comparison with the flexible Li-ion battery indicated inferior environmental performance of the all-organic battery due to its relatively low specific energy (Wh/kg) and large amount of materials needed for production of its electrode backbones. Sensitivity analysis showed that changing scaling-up parameters and the production route of 3,4-ethylenedioxythiophene (a precursor of electrode backbones) strongly influenced the results. In order to lower the environmental impacts of the all-organic battery, future research should focus on designing a short production chain with lower material inputs of electrode backbones, increasing battery cycle life, and improving the specific energy of the battery. In addition, relevant recommendations were provided for prospective LCAs of upscaled systems.

1. Introduction

In recent years, flexible electronics with potential applications as wearable devices, environmental sensors, flexible displays, or soft robots have attracted a great deal of research and market attention (Mackanic et al., 2020; Wehner et al., 2021). Use of these flexible devices can provide a better user experience, facilitate sustainability and health, and improve the connectivity of humans. However, such flexibility cannot be achieved using conventional batteries, designed as multilayer structures using stiff battery materials (Qian et al., 2019). To achieve the flexibility needed, extensive research has been performed to identify bendable and lightweight batteries as power sources for future flexible electronics (Wehner et al., 2021).

Two general approaches available to introduce flexibility in batteries are: 1) to process conventional stiff battery materials into flexible structures or 2) to replace the stiff materials with soft and bendable materials. Using these approaches, many flexible battery technologies, such as flexible Li-ion batteries, flexible lithium sulfur (Li/S) batteries, flexible zinc ion batteries (ZIB), and emerging organic batteries, have been developed, based on modifying conventional battery materials and structures (Wehner et al., 2021). Li-ion batteries are considered a promising power source for future flexible electronics, due to their high energy and power density, and favorable cycle life (Fang et al., 2020). The high theoretical capacity of Li/S and low cost of ZIB are the main features attracting research attention for future flexible electronics applications. However, long-term cycling stability for Li/S batteries remains an obstacle to further implementation, while a flexible configuration of ZIB has not yet been satisfactorily achieved (Gao et al., 2021; Yu et al., 2019). Using inorganic battery materials also creates environmental issues, such as mineral scarcity, ecotoxicity and human toxicity caused by metal mining, and geo- and socio-political problems (e.g., cobalt mining-related issues) (Larcher and Tarascon, 2015; Muench et al., 2016).

Compared with inorganic batteries such as Li-ion batteries, Li/S, and ZIB, organic battery materials have intrinsic advantages such as

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Abbreviations and nomenclature

Abbreviations

LCA	Life cycle assessment
Li-ion	Lithium-ion
Li/S	Lithium sulfur
ZIB	Zinc ion battery
TRL	Technology readiness level
FU	Functional unit
DoD	Depth of discharge
LTO	$Li_4Ti_5O_{12}$/Lithium Titanate Oxide
PDMS	Polydimethylsiloxane
$Pd(PPh_3)_4$	Tetrakis(triphenylphosphine)palladium(0)
$CHCl_3$	Trichloromethane
CNT	Carbon nanotube
EDOT	3,4-Ethylenedioxythiophene
ProDOT	3,4-propylenedioxythiophene
pEP(QH_2)E	p refers to polymerized, E to 3,4-ethylenedioxythiophene, P to 3,4- propylenedioxythiophene, QH2 to hydroquinone
pEP(NQ)E	p refers to polymerized, E to 3,4-ethylenedioxythiophene, P to 3,4-propylenedioxythiophene, NQ to naphthoquinone
EOL	End-of-life

Nomenclature

T_f	A future point in time
T_0	Present time

flexibility in configuration, synthetic tenability, relatively low reaction temperature, and low energy requirement in production processes (Kim et al., 2017; Muench et al., 2016). Organic battery materials may also become extractable from abundant biomass resources. A major challenge with organic battery materials is electrode dissolution, but this can be resolved using conductive redox polymers, formed by attaching redox-active pendant groups to conductive polymer backbones (Muench et al., 2016), as electrode material. A state-of-the-art all-organic battery using quinones as pendant groups and 3,4-propylenedioxythiophene-based polymers as backbones was developed recently (Strietzel et al., 2020). Compared with other organic batteries, it uses no additives and binders in electrode materials, which simplifies battery structure and manufacture (Hager et al., 2020; Muench et al., 2016). It can also be made using different substrate and coating methods, facilitating industrial-scale manufacturing.

There has been considerable market interest and much research on flexible battery technologies, but there has been a lack of research on the environmental impact of flexible batteries, especially organic batteries made using emerging materials. To our knowledge, only one study has assessed the environmental impacts of all-organic batteries using life cycle assessment (LCA), based on laboratory-scale production (Zhang et al., 2022). Uncertainty and limitations of using LCA results based on laboratory data to guide sustainable development of emerging technologies have been discussed previously (Hetherington et al., 2014). When small-scale production processes are scaled up, the efficiency gain in materials and energy use will likely reduce the overall environmental impact, and also change or uncover environmental hotspots. Therefore, a prospective LCA is needed to assess potential environmental impacts at a future point in time (T_f) when the battery technology reaches its full-scale operation. Prospective LCA considers possible changes in a system (foreground and background system) from present time (T_0) to T_f (Arvidsson et al., 2018). Such changes occur at: i) production process level, e.g., changes in production routes, raw materials, energy and material use efficiency, yield, etc.; and ii) technology performance level, e.g., changes related to the function of the technology.

The objectives of this study were to: (1) explore potential future environmental impacts of a state-of-the-art all-organic battery at industrial production scale; (2) compare the environmental performance of the all-organic battery with that of a flexible Li-ion battery, using prospective LCA; and (3) formulate environmental impact-related recommendations for future development of the all-organic battery. To our knowledge, this is the first environmental assessment of flexible batteries at industrial scale. The results can serve as early guidance for sustainable development of all-organic battery technology to prevent unintentional future environmental consequences, and act as a benchmark for later LCA studies in flexible battery technologies.

2. Material and methods

The methodological framework applied is shown in Fig. 1. The current processing steps for organic batteries and Li-ion batteries are laboratory-based, so their technology readiness level (TRL) is similar (around 4) (see T_0 in Fig. 1). A predictive scenario combined with a scaling-up method was used to scale up the battery technology system from laboratory-scale production (T_0) to industrial scale (T_f) (Fig. 1).

It took 12 years to develop traditional Li-ion batteries from innovation to sufficient maturity for industrial-scale production (TRL = 9) (Gross et al., 2018). Using this as reference, while considering the consistently increasing speed of innovation and commercialization of new electronics (Gross et al., 2018), it was assumed that the all-organic battery technology and flexible Li-ion battery technology could both reach maximum TRL within 10 years. This short-term scenario allowed reasonable direct use of current background data, without important changes (Arvidsson et al., 2018; Villares et al., 2017).

LCAs were conducted on the future battery production systems (T_f). The prospective LCA results obtained for the all-organic battery were compared with those for the flexible Li-ion battery, and also with those for the laboratory-scale LCA. Technical details of the two flexible battery systems studied are described in sections 2.2.1 and 2.2.2.

2.1. Goal and scope

The goal was to conduct prospective LCA on two flexible battery systems: an all-organic battery and a flexible Li-ion battery, to quantify the environmental impacts associated with the production of the all-organic battery and to compare its environmental performance to that of the flexible Li-ion battery. Since the focus was on battery production, a cradle-to-factory gate system boundary was used (Fig. 2). The functional unit (FU) selected was 1 kWh of energy delivered over the lifetime of the flexible battery cell. The battery life cycle was modeled using the database Ecoinvent 3.6 (cut-off). The system was modeled using SimaPro® software.

2.2. Life cycle inventory and data sources

2.2.1. All-organic battery technology

The all-organic battery assessed was that developed by Strietzel et al. (2020). Fig. 3a shows the composition of the all-organic battery cell. The anode and cathode consist of the newly developed conductive redox polymer materials pEP(QH_2)E and pEP(NQ)E, with trimeric thiophene repeating units (EPE) as backbones and quinone-based pendant groups (QH_2 and NQ). The electrolyte is 0.5 M H_2SO_4 (aq) and Asahi TU-10S carbon conductive paste is used as the current collector in the laboratory-scale battery. Due to lack of data, graphite was used as a proxy for the latter in the present analysis. A glass microfiber filter is used as separator and Dupont FEP 500C film as the battery casing in the laboratory-scale battery. Due to lack of data, in the LCA model the latter was replaced with a commonly used flexible battery casing, polydimethylsiloxane (PDMS) (Mackanic et al., 2020; Zhou et al., 2021). A lifetime of 1000 cycles and average depth of discharge (DoD) of 80%

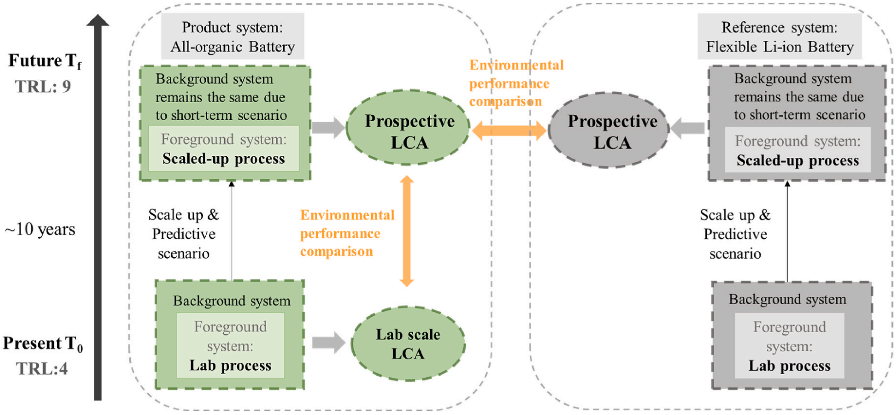

Fig. 1. Methodological framework applied in this study. The all-organic battery production system is shown in green and the flexible Li-ion battery system in gray. Rectangles depict battery systems and ovals depict LCA models. The black arrow on the extreme left represents the timeline, with present time (T_0) at the bottom and future time (T_f), when the battery system has reached its highest technology readiness level (TRL), at the top.

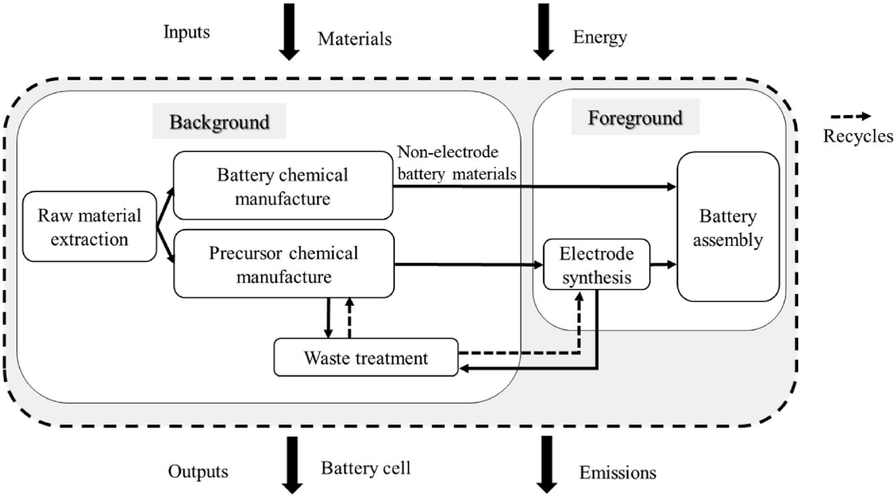

Fig. 2. Flowchart showing process steps and the system boundary applied in prospective life cycle assessment (LCA) of production of an all-organic battery. The system boundary includes foreground processes and background processes.

were assumed in each charge-discharge cycle for the all-organic battery. Details of electrode production, relevant calculations, and assumptions are given in SM (part S1.2) and technical details in Table 1. The production chain of the all-organic battery was divided into seven production stages, based on the chemical structure of the electrode active materials (backbone and pendant group): production of anode backbone, production of anode pendant group, production of anode, production of cathode backbone, production of cathode pendant group, production of cathode, and production of non-electrode components.

2.2.2. *Flexible Li-ion battery technology*

To gain a better understanding of the all-organic battery system, a flexible Li-ion battery was selected as reference (Hu et al., 2010). In addition to its lightweight and high performance characteristics, the flexible Li-ion battery has a simple and cheap synthesis process and all battery materials are highly commercialized compared with those in other flexible metal-ion battery technologies (Mackanic et al., 2020; Wehner et al., 2021).

In the flexible Li-ion battery composition (Fig. 3b), $Li_4Ti_5O_{12}$ (LTO) and $LiCoO_2$ (LCO) were used as anode and cathode active materials, respectively. A sheet of commercial paper was used as the separator and a highly conductive carbon nanotube film as the current collector for the anode and the cathode. The battery cell was assumed to be sealed with PDMS using $LiPF_6$-based electrolyte. A lifetime of 4000 charging cycles has been reported for a conventionally designed LCO/LTO battery system (Majima et al., 2001). This was assumed to be a feasible cycle life for

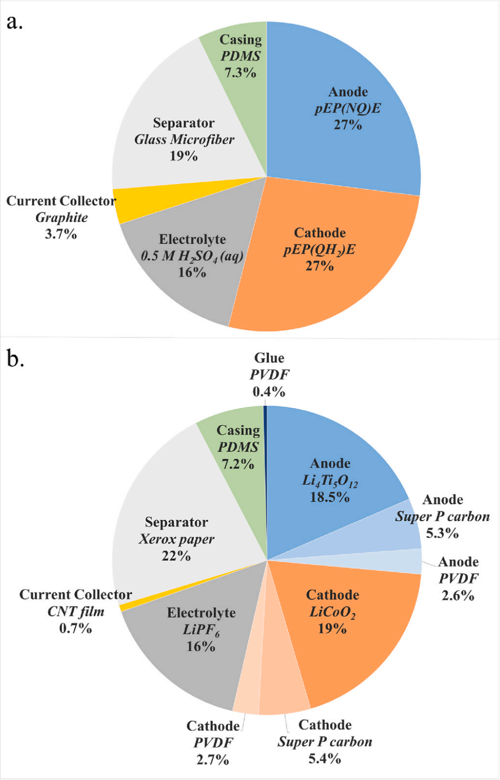

Fig. 3. Composition (wt-%) of the all-organic battery (a) and the Li-ion battery (b).

Table 1
Technical details of two flexible battery cells.

	All-organic battery	Flexible Li-ion battery
Size assessed in this study	3 cm × 3 cm	3 cm × 3 cm
Weight	243.4 mg	245 mg
Voltage	1 V	2.7 V
Specific energy	21.6 Wh/kg	108 Wh/kg
Lifetime (charge-discharge cycles)	1000	4000
Depth of discharge, DOD	80%	80%
Technology readiness level: battery technology	4	4
Technology readiness level: battery materials	Electrodes: 3-4 Non-electrodes: 9	9

the studied flexible Li-ion battery. An average DoD of 80% was assumed in each charge-discharge cycle. Detailed assumptions are presented in SM (part S1.1) and other technical details in Table 1.

2.2.3. Data collection

For foreground system processes of the studied all-organic battery, electrode production is still in an early development stage, which means that no large-scale production data is available. Laboratory-scale production processes of electrodes, which comprise many chemical synthesis steps, were provided by the Nanotechnology and Functional Materials group at Uppsala University. Each synthesis step was scaled up based on parameters provided by Geisler et al. (2004) and Capello et al. (2005). Geisler et al. (2004) established the best- and worst-case parameter values for calculating material and energy flows required in LCIs of producing fine and specialty chemicals (Table S2.1). These best- and worst-case parameters are estimated using on-site data from large-size plant processes and pilot plant processes, separately. Considering that neither the best- nor worst-case parameters can represent the average-size plant processes, this study calculated the average values of these two as scaling-up factors for each synthesis step (Table S2.1). For reaction yield, a value of 0.95 was used rather than the average value since it is commonly used in previous study and Ecoinvent database (Althaus et al., 2007; Wernet et al., 2012). Waste solvents generated from each synthesis step (or unit process) were treated by distillation and reused in the same process, which was modeled using parameters provided by Capello et al. (2005) (Table S2.1). The influence of using average parameter values was tested in the sensitivity analysis. LCI data on non-electrode components were collected from Ecoinvent 3.6 database. A detailed inventory can be found in Tables S2.17-S2.22.

For background system processes, the inventory was based on a laboratory-scale LCA of the same all-organic battery (Zhang et al., 2022), but with some refinements. The modified inventory is provided in Tables S2.11-S2.16. Input and output data from background system were obtained from the Ecoinvent 3.6 database whenever possible. Data not available in the Ecoinvent database were generated by establishing production routes based on information from patents and literature. The LCI was further completed using utility inputs calculated with parameters taken from the literature (Capello et al., 2005; Piccinno et al., 2016). While the raw materials for producing the all-organic battery can theoretically be extracted from biomass, appropriate synthesis processes still require extensive studies and development. Therefore, fossil-based raw materials were used in the model.

For wider development of all-organic battery technologies, it is crucial to consider the scalability and recyclability of relevant resources. $Pd(PPh_3)_4$ is used as a homogeneous catalyst for producing electrode backbones and could be a bottleneck for upscaling due to its high cost. Previous studies have shown that $Pd(PPh_3)_4$ can be recycled and reused efficiently following nanofiltration (Gursel et al., 2015; Janssen et al., 2011). Therefore, in the present analysis it was assumed that nanofiltration was used for recycling the Pd catalyst and that the recycled catalyst was reused. As a result, $Pd(PPh_3)_4$ usage per FU was too small to make a significant contribution, and was therefore not included in the model. Use of secondary metals in the final fabricated metal was considered for copper (Cu) and zinc (Zn). Copper components were considered to comprise 68% primary and 32% secondary Cu, while Zn components were considered to comprise 70% primary and 30% secondary Zn (Graedel et al., 2011; Norgate, 2013).

The flexible Li-ion battery was modeled using industrial-scale data. Input and output data were obtained from the Ecoinvent 3.6 database, whenever possible. Data not available in Ecoinvent were derived from best available literature data (see Tables S2.2-S2.10). For both flexible battery systems, Swedish and European data from the Ecoinvent 3.6 database were used when available. Otherwise, global data were used. Electricity mix used in the study is modeled as Swedish electricity mixture from year 2014 (approximately 47% of hydro, 37% of nuclear, 11% wind, 3% biomass).

2.3. Life cycle impact assessment (LCIA)

The ILCD 2011 midpoint method was used to quantify environmental impacts (Hauschild et al., 2011). The most significant impact categories were selected based on the normalized and weighted LCA results as those with a cumulative contribution of more than 80% to the total environmental impacts (Table S3.1), without considering toxicity-related categories (European Commission, 2018). The following impact categories were considered: mineral, fossil, and renewable resource depletion (in kg Sb-eq); climate change (in kg CO_2-eq); ozone depletion (in kg CFC-11-eq); and ionizing radiation (in kBq U235-eq). In order to get a complete overview of the environmental performance, three toxicity-related impact categories were also included: freshwater ecotoxicity (in CTUe), human toxicity with cancer effects (in CTUh), and human toxicity with non-cancer effects (in CTUh). Cumulative energy demand was used to calculate the primary energy requirement along the life cycle of the two battery types.

3. Results and discussion

3.1. Environmental profile of an all-organic battery

The environmental impacts per FU in the selected impact categories from industrial production of the all-organic battery are shown in Table 2 and the environmental impacts in all impact categories of the ILCD 2011 midpoint method are shown in Table S3.2. Overall, electrodes (>91%) were the most influential battery components for the selected impact categories, with the cathode (45–66%) showing higher environmental impacts than the anode (33–46%) (Table 2). This was due to the long production route of the cathode backbone, resulting in high chemical material consumption and associated high waste volumes. Among the production stages, production of the electrode backbones was the greatest contributor (60–87%) to the total impacts at industrial scale (Table 2). Overall, EDOT, a precursor of electrode backbones, was the largest contributor, accounting for 21–59% of the total impacts for the selected impact categories (Table S4.1).

Fig. 4 summarize the main contributors for different impact categories. Catalysts used in upstream systems were the dominant contributors to resource depletion, human toxicity non-cancer effects, and freshwater ecotoxicity as environmental impacts of organic batteries in industrial-scale production (Fig. 4). NH_3Cl/Zn, a reducing catalyst used for producing 3,4-dibromothiophene (EDOT precursor), was the largest single contributor to resource depletion potential (78%). Zinc also had a great influence on human toxicity with non-cancer effects (18%) and freshwater toxicity (9%). Copper oxide, used as a catalyst for producing 3,4-dimethoxythiophene (a precursor for electrode backbones), accounted for 46% and 23% of human toxicity with non-cancer effects and freshwater ecotoxicity, respectively. These toxicity-related environmental impacts mainly derived from Zn and Cu mining activities, e.g., Cu leaching from sulfuric tailings generated in Cu mining and sulfate, Zn, cadmium, and other metals released from Zn mining. These emissions can move into groundwater and soils, directly or indirectly affecting human health and causing water pollution (Song et al., 2017; Zhang et al., 2012). Other catalysts such as $SnCl_2$, used in production of 2,5-dihydroxybenzaldehyde (precursor of cathode pendant group), accounted for 10% of the resource depletion potential. The environmental impacts of $SnCl_2$ in other impact categories were minor (<1%).

Solvents were the dominant contributors (89%) to ozone depletion potential (Fig. 4). Trichloromethane ($CHCl_3$) were the most significant contributor, accounting for 74% of the total ozone depletion potential impact. Most of the $CHCl_3$ (>73%) was used for producing 3,4-dibromothiophene (a precursor for EDOT). DCM (5% contribution) was used as a solvent in different chemical reactions and purification processes along the production chain. The ozone depletion caused by use of $CHCl_3$ is due to carbon tetrachloride (CCl_4) emissions during production of $CHCl_3$. It has been shown that use of $CHCl_3$ may delay recovery of the Antarctic ozone layer (Fang et al., 2019). Use of solvents also had a major influence on climate change (16%), human toxicity with (12%) and without (14%) cancer effects, freshwater ecotoxicity (12%), and ionizing radiation (9%).

Waste treatment processes not only emitted large amounts of greenhouse gases but also led to the release of toxic chemicals, e.g., Cr (VI)), into air, soil, and water, directly and indirectly affecting human health (Kapoor et al., 2022). Consequently, waste treatment processes were the greatest contributors to global warming potential (37%) and human toxicity with cancer effects (53%), and played a main role in human toxicity without cancer effects (15%), freshwater ecotoxicity (13%), and ionizing radiation (6%).

Energy consumption was the main contributor to ionizing radiation (50%), mainly due to use of uranium for nuclear-based electricity production, and a major contributor to climate change (15%). Bromine, a reagent used for producing intermediate chemicals in both the background and foreground systems, contributed 10% to climate change and 8% to human toxicity with non-cancer effects. Production of bromine requires a large amount of heat, and processes related to hard coal mining, combustion, and waste treatment emissions affect the environment and human health.

Environmental impacts of the all-organic battery were reduced by 97–99% when comparing prospective LCA results with laboratory-scale LCA, for the most significant impact categories (Tables S3.4-3.5). This was mainly due to improved solvent use efficiency, reduced amounts of waste, and reuse of catalysts (Table S3.6). Previous studies have shown that total environmental burden is often reduced on upscaling production systems, because of material and energy efficiency gains, recycling of feedstock, and enhanced yield (Gavankar et al., 2015; Piccinno et al., 2016). Such efficiency improvements resulted in a significant change in the relative environmental contribution of material and energy flows to total environmental impacts of the all-organic battery, as shown by comparison of environmental hotspots at industrial (Fig. 4) and laboratory scale (Fig. S2). This indicates that laboratory-scale LCA can produce misleading results when used for identifying environmental hotspots of emerging technologies. In order to increase the robustness of prospective LCAs, potential changes in key environmental contributors during upscaling should thus always be considered in such LCAs. Based on previous studies, particular attention should be devoted to process flows that show marked reductions during upscaling, such as solvents (Pallas et al., 2020b; Piccinno et al., 2018), energy (Gavankar et al.,

Table 2

Prospective life cycle assessment characterization results and contributions from different production stages to the overall impacts for each impact category using the FU of 1 kWh energy provided over the lifetime of an all-organic battery cell. (Stage I = production of anode backbone, Stage II = production of anode pendant group, Stage III = production of anode, Stage IV = production of cathode backbone, Stage V = production of cathode pendant group, Stage VI = production of cathode, Stage VII = non-electrode component production.)

Impact category	Value (per FU)	Percentage by production stage						
		Anode			Cathode			Non-electrode components
		Stage I	Stage II	Stage III	Stage IV	Stage V	Stage VI	Stage VII
Climate change	8.2 kg CO_2-eq	22%	2%	9%	46%	15%	5%	1%
Ozone depletion	5.3×10^{-5} kg CFC-11-eq	26%	1%	20%	42%	0%	2%	9%
Human toxicity, non-cancer effects	1.7×10^{-6} CTUh	27%	2%	6%	48%	11%	3%	2%
Human toxicity, cancer effects	4.9×10^{-7} CTUh	21%	3%	9%	45%	16%	5%	1%
Ionizing radiation HH	0.7 kBq U235-eq	21%	7%	7%	39%	14%	4%	8%
Freshwater ecotoxicity	1×10^{2} CTUe	27%	2%	6%	51%	11%	2%	1%
Mineral, fossil & renewable resource depletion	1×10^{-3} kg Sb-eq	35%	0%	1%	52%	11%	1%	0%

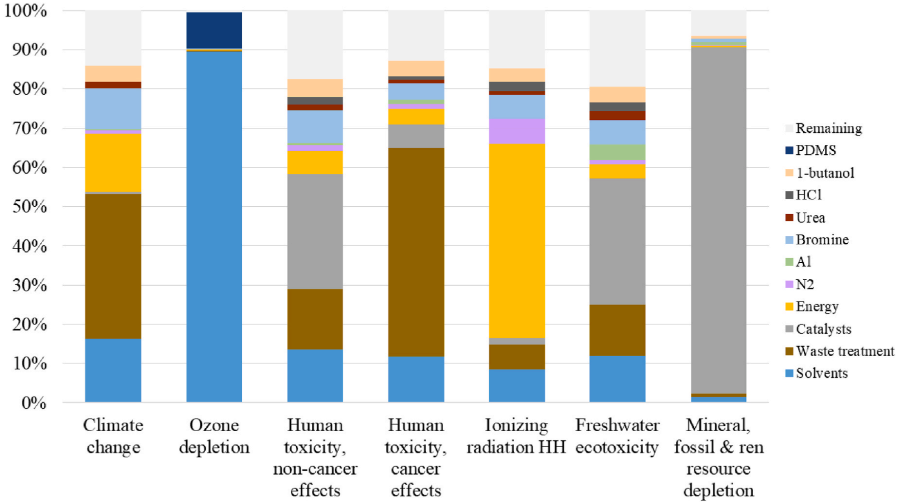

Fig. 4. Relative contribution of different process flows in industrial-scale production of organic batteries to the most significant impact categories.

2015; Piccinno et al., 2015), and materials that are likely to be recycled in mass production, e.g., metals (Pallas et al., 2020a; Villares et al., 2017). Additionally, 3–10% of the environmental impact reduction was attributable to changes in all-organic battery composition and improvements in battery performance, suggesting that it is necessary to consider technological development in prospective LCAs.

3.2. Comparison with flexible Li-ion battery

3.2.1. Primary energy consumption

Life cycle cumulative energy demand (CED) calculated the direct and indirect energy use throughout the life cycle of two flexible batteries. Direct energy use refers to energy needed in the battery processing steps, including the electrode manufacturing, cell assemble, and cell formation. Indirect energy use refers to energy embedded in raw materials. Based on the FU of 1 kWh of energy delivered over the lifetime of the batteries, the CED in production of the all-organic battery (125 MJ) was 2.7-fold higher than that in production of the flexible Li-ion battery (46 MJ). This was partly due to the low specific energy and short cycle life of the all-organic battery. Another reason was that the long production chain of the all-organic battery required large amounts of materials, resulting in a high amount of embedded energy. In production of the all-organic battery, 98% of the energy requirement was attributable to the electrodes, with anode and cathode backbone production requiring 64% of total energy, while less than 1% of the energy requirement was associated with battery material coating and battery assembly processes. The CED for the flexible Li-ion battery was dominated by the carbon nanotube (98%) used as current collector in the battery cell, due to the large amount of energy required in its production and purification (up to 8.7×10^7 MJ/kg of product) (Upadhyayula et al., 2012). Note that electricity consumed for charging the batteries was not considered, since the focus was on battery production.

3.2.2. Selected impact categories

The prospective LCA results for the two flexible battery types were compared using the flexible Li-ion battery as the basis for normalization (Table 3). The environmental impacts per FU from industrial production of the flexible Li-ion battery are shown in Table S3.3. The impact of different lifetimes of the all-organic battery (1000, 2000, and 4000 charge-discharge cycles) was considered in the comparison, since the lifetime of all-organic batteries is uncertain. For all selected environmental impact categories except ionizing radiation, the all-organic battery showed higher environmental impacts than the flexible Li-ion battery even when both had the same lifetime (4000 cycles) (Table 3). The relatively high ionizing radiation of the flexible Li-ion battery was due to 37% of the primary energy in battery production coming from nuclear power. Surprisingly, production of the all-organic battery had higher impacts on resource depletion, although no metal was used directly in battery components. This was due to metallic catalysts being used in several chemical reaction steps in the upstream system. Large amounts of material were required per FU in the upstream system due to material losses throughout the production chain. For example, 4.76 g of Zn, 0.87 g of Cu, and 0.21 g of Sb were needed for production of the all-organic battery (with a lifetime of 4000 cycles), while only 0.46 g Co, 0.12 g Li, and 0.74 g Ti were required for production of the flexible Li-ion battery (also with a lifetime of 4000 cycles).

Table 3
Comparison of environmental performance of the flexible Li-ion battery and of all-organic batteries with different cycle lifes (1000, 2000, 4000 charge-discharge cycles).

Impact category	Li-ion_4000	All-organic battery_1000	All-organic battery_2000	All-organic battery_4000
Climate change	1	20	10	5
Ozone depletion	1	114	57	28
Human toxicity, non-cancer effects	1	8	4	2
Human toxicity, cancer effects	1	15	8	4
Ionizing radiation HH	1	0.3	0.2	0.1
Freshwater ecotoxicity	1	7	3	2
Mineral, fossil & renewable resource depletion	1	29	14	7

Increasing battery lifetime from 1000 to 4000 charge-discharge cycles significantly reduced the environmental impacts of the all-organic battery, but still resulted in higher environmental impacts than for the flexible Li-ion battery (Table 3). One main reason was that the specific energy of the all-organic battery cell (21.6 Wh/kg) was 5-fold lower than that of the flexible Li-ion battery (108 Wh/kg) on a mass basis, which meant that more bulky organic batteries were needed to deliver the same amount of energy. Even though all-organic battery technology was assumed here to be designed for small portable devices, where high specific energy is not the only target, the low specific energy will certainly limit its future applications.

3.3. *Sensitivity analysis and uncertainties*

Six aspects identified as having strong potential impacts on the results were tested and discussed in sensitivity analysis. These were: 1) scaling up method; 2) EDOT production route; 3) replacing brominated aromatic hydrocarbons with chlorinated aromatic hydrocarbons; 4) battery design of the all-organic battery; 5) resource scarcity measurement method; 6) considering end-of-life processes in the system boundary.

3.3.1. *Impact of scaling-up method*

Parameters used to scale up LCIs of laboratory-scale electrode production were tested in the sensitivity analysis, with average parameter values as the baseline scenario. Best- and worst-case scenarios were established using best- and worst-case parameters estimated based on on-site data from large plant processes and pilot processes, separately (Table S2.1). The results show that the changing scaling-up parameters can affect the environmental impacts considerably (Fig. 5). Compared with baseline scenario, applying best-case scenario reduced 10–38% of environmental impacts, while applying worst-case scenario increased 60–136% of the environmental impacts. For reference, previous study also showed that existing industrial processes correspond more frequently to the best-case parameters rather than the worst-case parameters (Geisler et al., 2004).

Another uncertainty of the scaling-up method is that the electrode production route will most likely be optimized for large-scale production. According to battery developers, the production chain certainly will be shorter, due to economic considerations, when the all-organic battery electrodes are produced at industrial scale. Consequently, the prospective LCA results for the all-organic battery are possibly overestimates of the environmental impacts. However, such production chain optimization requires further extensive research, and such uncertainty cannot be assessed at the current development stage. As previous study suggested that a new LCA study should be performed when there is major change in the production chain (Pallas et al., 2020b).

3.3.2. *Impact of alternative EDOT production route*

Another production route for EDOT, based on Roes et al. (2009), was modeled to study the effect of an alternative synthesis method on the total environmental impacts (Table S4.2). The results showed that changing the EDOT production method increased the ionizing radiation potential impact by 99%, while total impacts in other impact categories decreased by 17–59% (Fig. 6). Despite this reduction, production of the electrode backbones still proved to be a key contributor, accounting for 42–80% of the total impacts (Table S4.3).

The sensitivity analysis thus indicated a need to consider uncertainties involved in choice of chemical production route in the LCA model. New or uncommon materials, which are usually not included in LCA databases, are often used in emerging technologies (Hetherington et al., 2014). Establishing a LCI for new material by identifying its production route based on information from patents or scientific papers is a recommended way to deal with data gaps (Arvidsson et al., 2014). In fact, a multitude of alternative synthesis routes commonly exist for a given chemical, and the environmental impacts can vary between these synthesis routes. For example, Arvidsson et al. (2014) showed that the environmental impacts of graphene vary considerably depending on the production route used.

3.3.3. *Impacts of different resource scarcity measurement methods*

Resource scarcity can be measured with various methods. In this study it was modeled using the abiotic depletion method, which measures scarcity by including extractions and reserves of a given resource. In sensitivity analysis, the surplus ore potential method was used to test the effect of different resource scarcity assessment methods on the results. Table 4 shows the LCA results for all-organic flexible batteries with two different cycle lifes, normalized using the flexible Li-ion battery as a basis. As can be seen, production of the all-organic battery still resulted in higher resource depletion impacts than production of the flexible Li-ion battery, although the relative impact was reduced.

3.3.4. *Replacing Br_2 with Cl_2*

In theory, halogenated aromatic hydrocarbons share similar chemical properties. According to the Ecoinvent 3.6, production of chlorine has lower environmental impacts than production of bromine for most environmental impact categories. Therefore, in sensitivity analysis

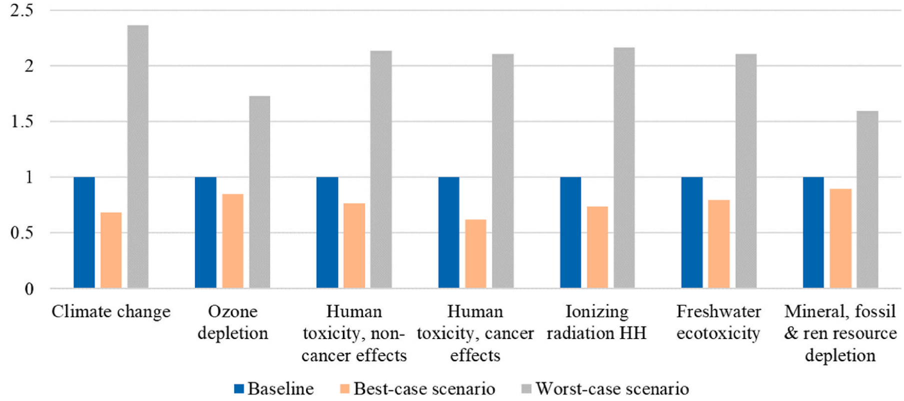

Fig. 5. Influence of scaling up parameters.

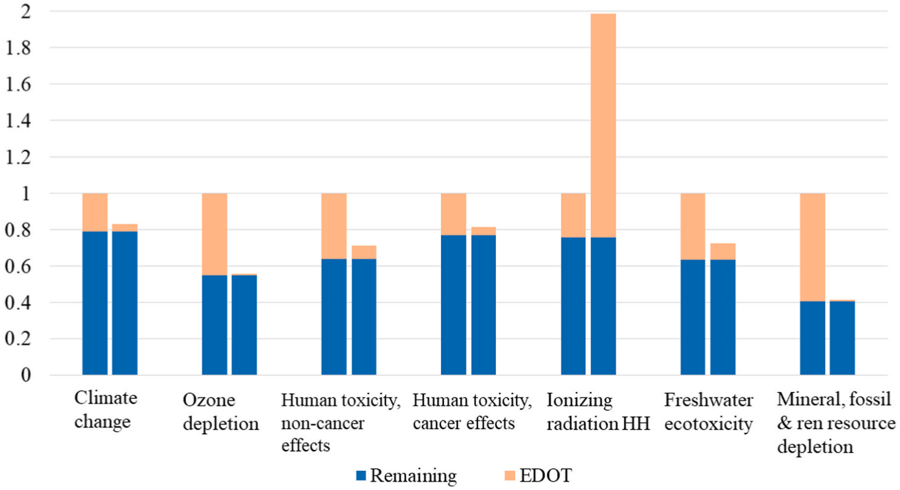

Fig. 6. Effect of changing 3,4-ethylenedioxythiophene (EDOT) production route on the environmental impact in significant impact categories assessed in this study. For each impact category, the left column refers to the baseline LCA result, while the right column refers to the LCA result after changing the EDOT production route.

Table 4
Effect of different resource scarcity measurement methods on the resource depletion environmental impact of the flexible Li-ion battery and of all-organic batteries with different cycle lifes (1000, 4000 charge-discharge cycles).

	Method	Flexible Li-ion battery_4000	All-organic battery_1000	All-organic battery_4000
ILCD Midpoint (2011)	Abiotic depletion method	1	29	7
ReCiPe 2016 Midpoint (H) V1.04	Surplus ore potential method	1	18	4

brominated aromatic hydrocarbons (Br_2ProDOT-OH) used in production of the all-organic battery cells were assumed to be replaced with chlorinated aromatic hydrocarbons (Cl_2ProDOT-OH) (Fig. S1). The results showed that changing the raw material from Br_2 to Cl_2 reduced the total environmental impacts for the selected environmental impact categories by 4–6%.

3.3.5. Impact of battery design

Since the current laboratory data cannot reflect industrial production, the mass of battery components used in all-organic battery cells was adjusted using the flexible Li-ion battery as reference. To test how this assumption affected the results, in sensitivity analysis the mass ratio of the battery components in a commercial pouch Li-ion cell (Golubkov et al., 2014) was used instead to reconstruct the all-organic battery (Table S4.4). Pouch cell design was selected because it can still partly retain the flexibility of the all-organic battery, despite its multilayer structure. The results showed that the environmental impacts were reduced by 1–24% for the selected environmental impact categories (Fig. 7). This was because the proportion of electrode active materials in

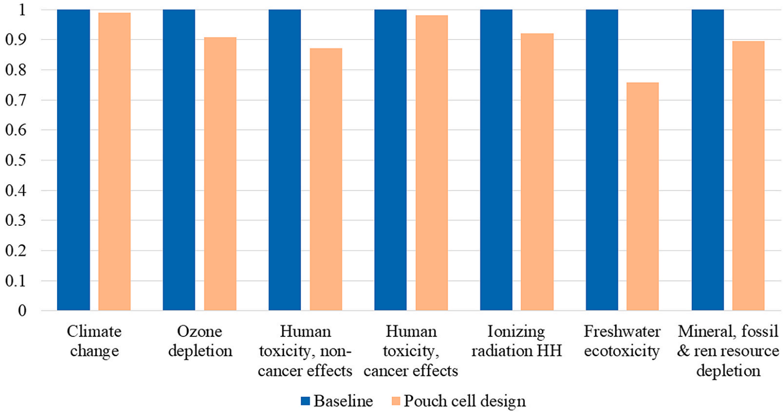

Fig. 7. Effect of changing battery design on the environmental impact in significant impact categories assessed in this study.

the pouch cell was higher, resulting in higher specific energy and requiring less battery materials per FU. However, it should be noted that this reduction in environmental impacts was at the expense of configuration flexibility.

3.3.6. *Impact of excluding end-of-life stage*

End-of-life (EOL) processes were not included in the system boundary since the focus was on battery production. The influence of excluding the EOL stage on the results of the included impact categories was assessed in the sensitivity analysis. The EOL of organic batteries can be disposed of or incinerated in the same way as the product in which they are integrated, due to the absence of metals in battery materials. Therefore, three different waste treatment methods from Ecoinvent 3.6 were used as EOL treatment scenarios: (1) Treatment of packaging waste; (2) Treatment of municipal solid waste, incineration; (3) Treatment of municipal solid waste, landfill. Results revealed that including EOL processes have minor changes ($<1\%$) for all impact categories except freshwater ecotoxicity (increased 3–5%) and human toxicity with non-cancer effects (increased 4–6%) (Table S4.5).

As for the flexible Li-ion battery, it was found that closed-loop recycling of Li-ion battery materials can result in significant environmental benefits (Jiang et al., 2022). Wu et al. (2022) found that up to 261 kg CO_2-eq emissions can be offset when regenerating 1 kg of LCO. However, it is worth noting that several obstacles regarding recycling Li-ion batteries still need to be overcome, e.g. safety issues caused by not fully discharged batteries (Bauer et al., 2022); human and environmental toxicity caused by possible informal recycling (Zhang et al., 2021); and lack of management involvement in the used battery collection (Jiang et al., 2021).

The above-discussed information indicated that including EOL in the system boundary can increase the difference in environmental performance between the two batteries. Considering the inferior environmental performance of the all-organic battery compared to that of the Li-ion battery, as well as the easy EOL treatment of the all-organic battery, we suggest that future applications of all-organic batteries should focus on special fields where the battery is difficult to remove and recycle.

3.4. *Opportunity for improvements*

Environmental hotspots identified and the results from sensitivity analysis can provide important information to researchers and technology developers on how to improve the environmental performance of emerging technologies. Based on findings in this study, future research efforts on the all-organic battery should focus on reducing the environmental impacts from production of the electrode backbones, e.g., by developing or implementing a suitable synthesis route with less input of materials, developing a synthesis route with fewer synthesis steps, or designing an alternative lightweight backbone structure. Increasing the cycle life (number of charge-discharge cycles) could also reduce the environmental impacts of all-organic batteries. Further, use of materials with lower environmental impacts should be explored, to allow replacement of materials with high environmental impacts, e.g., chlorinated aromatic hydrocarbons are a more environmentally friendly alternative to brominated aromatic hydrocarbons when halogenated aromatic hydrocarbons are needed for a reaction. Moreover, increasing the specific energy of the battery, by e.g., increasing the mass loading of electrode active material or using light and sustainable materials for non-electrode materials, could reduce the environmental impacts. Changing to a pouch cell design could also reduce environmental impacts, this could decrease the flexibility of the battery, a trade-off which has to be considered by battery developers.

This study found that TRL fails to provide accurate information on the maturity of technologies, especially for complex systems. This aspect is explained below and a potential solution for improvement is suggested. In reality, technologies with the same TRL might include components with different TRLs. In the case of the two battery production systems assessed in this study, both battery technologies had the same TRL (4), but the TRL of the battery materials differed, with electrode materials of the all-organic battery having significantly lower TRL (around 3–4) than that of the flexible Li-ion battery cell (TRL of 9 +). If such differences in TRL of the technology components are not specifically considered in comparisons from an LCA perspective, this may result in misleading recommendations. Therefore, we suggest that it is essential to illustrate not only the technology's TRL but also the TRL of the components used in the assessed technology, especially in comparative LCA. This can provide a better understanding of the performance of the emerging technology compared with that of established technologies.

4. Conclusions

This study assessed the potential environmental impacts of an all-organic battery at an industrial-scale production, based on 1 kWh of energy delivered over an assumed lifetime of 1000 cycles. The results showed that the production of anode and cathode had the greatest environmental impacts, with electrode backbones being the main contributors. The comparison with the flexible Li-ion battery indicated that the all-organic battery had higher impacts in most environmental impact categories assessed. The large uncertainties in future battery performance (e.g. cycle life), future production route, and production size indicated that an optimization potential can be expected for the all-organic battery and a better environmental performance can be achieved. In addition, the above-mentioned uncertainties need to be considered when results are used for benchmarking later LCA studies.

Following the findings of this study, future research on the all-organic battery should focus on increasing battery cycle life, optimizing production of electrode backbones by designing shorter synthesis routes with less material inputs, exploring sustainable alternative raw materials (e.g., replacing brominated aromatic hydrocarbons with chlorinated aromatic hydrocarbons), and designing a simplified backbone structure. In addition, increasing mass loading of electrode active materials, and reducing the weight of non-electrode materials, would also reduce the environmental impacts per kWh of energy delivered over lifetime.

Based on experiences gained during this research, the following recommendations are made for LCA of emerging technologies: 1) potential changes in environmental hotspots during scaling up should always be discussed in laboratory-scale LCAs; 2) potential changes in technology performance should be considered in prospective LCA; and 3) when using TRL to describe the maturity of a technology, the TRL of the technology itself and that of components embedded in the technology should be demonstrated, to provide a better understanding of the performance.

CRediT authorship contribution statement

Shan Zhang: Conceptualization, Methodology, Data curation, Formal analysis, Writing – original draft, Writing – review & editing. **Niclas Ericsson:** Conceptualization, Methodology, Writing – review & editing. **Martin Sjödin:** Supervision, Investigation, Writing – review & editing, Funding acquisition. **Hanna Karlsson Potter:** Supervision, Writing – review & editing. **Per-Anders Hansson:** Supervision, Conceptualization. **Åke Nordberg:** Supervision, Conceptualization, Writing – review & editing.

Declaration of competing interest

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.

Data availability

Data will be made available on request.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.jclepro.2022.133804.

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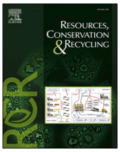

Future climate impacts of sodium-ion batteries

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ABSTRACT

Sodium-ion batteries (SIBs) have emerged as an alternative to lithium-ion batteries (LIBs) due to their promising performance in terms of battery cycle lifetime, safety, operating in wider temperature range, as well as the abundant and low-cost of sodium resources. This study evaluated the climate impacts of three SIBs, and compared to two LIBs under four scenarios with considering potential changes in battery performance and background productions between 2020 and 2050. To ensure a fair comparison, all batteries were modeled in the 21,700 form, and a battery dimensioning model was developed to calculate the required amount of components for each battery. We found that equal to lower GHG emissions result from the use of SIBs compared to LIBs under optimal performance scenarios. From 2020 to 2050, the climate impacts of SIBs decreased by 43–57 %. The relative contribution of the battery manufacturing process decreases from 18–32 % to 2–4 % due to the increasingly share of clean energy in the electricity grid, while the relative contribution of key battery component materials increases over time, especially for cathode active materials. These results emphasize the significance of decarbonizing the electric grid, and suggest that future investment in SIBs is promising from an environmental point of view.

Abbreviation

CMC	Carboxymethyl cellulose
DMC	Electrolyte: Dimethyl Carbonate
EC	Electrolyte: Ethylene Carbonate
EVs	Electric vehicles
G	Graphite
GHG	Greenhouse gas
HC	Hard carbon
IAM	Integrated assessment model
LCA	Life cycle assessment
LCI	Life cycle inventory
LFP	Lithium iron phosphate
LIB	Lithium ion battery
LMO	Lithium manganese oxides
NaPBA	Prussian blue analogues $Na_2FeFe(CN)_6$
NaPF6	sodium hexafluorophosphate
NMC811	Lithium nickel manganese cobalt oxide $LiNi_{0.8}Mn_{0.1}Co_{0.1}O_2$
NMMT	Sodium nickel manganese magnesium titanium oxide, $Na_{1.1}(Ni_{0.3}Mn_{0.5}Mg_{0.05}Ti_{0.05})O_2$
NMP	N-methylpyrrolidone
NVPF	polyanionic $Na_3V_2(PO_4)_2F_3$
PE/PP	polyethylene/polypropylene membrane
pLCA	prospective life cycle assessment
pLCI	prospective life cycle inventory
PVDF	Polyvinylidene fluoride
SBR	styrene butadiene rubber
SIB	Sodium-ion battery
VTM ore	vanadium-titanomagnetite ore

1. Introduction

Batteries play an essential role in the transition to a fossil-free society, as power sources for electric vehicles (EVs), and as storage technologies for intermittent renewable energies. International Energy Agency (IEA) predicted that battery demand for EVs could reach up to 5.6 TWh by 2030 (under Net Zero Emission scenario), which is 16 folds of the demand in 2021(IEA, 2022). Bogdanov et al. (2019) projected that 48 TWh of battery storage capacity is needed in order to achieve a 100 % renewable electricity system by 2050. Currently, lithium-ion batteries

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(LIBs) dominate the rechargeable battery market due to their versatility (covering a wide range of applications) and outstanding performance (e.g. high energy density, high power and good lifetime and energy conversion efficiency) (Kim et al., 2019). However, relying solely on LIBs to meet the fast-growing energy storage demand is putting significant pressure on lithium supply chain. This pressure could pose adverse effects on Indigenous people in mining regions (Owen et al., 2023), lead to ecosystem damage (Petavratzi et al., 2022), contribute to a serious lithium supply deficit (Greim et al., 2020), and consequently results in lithium prices increase (Tapia-Ruiz et al., 2021). The short-term availability concerns on lithium supply, in combination with the geographically-constrained reserves and inefficient resource management in the “lithium triangle” (the lithium reserves abundant region, concluding Bolivia, Chile and Argentina) (Eftekhari, 2019), have raised awareness on the importance of developing alternative battery technologies.

Meanwhile, the increasing amount of research on sodium-ion batteries (SIBs) and the growing numbers of SIB startups show that SIBs are attracting significant attention as a potential alternative to LIBs (Broux et al., 2019; Rudola et al., 2021a). Several companies, such as Faradion in UK (Faradion, 2022), CATL in China (Carla, 2023), Tiamat in France (Tiamat, 2022), Natron from the United States (Natron Energy, 2023), etc. have developed commercial prototypes. This is due to the abundance and low cost of sodium resources, the high safety and long cycle life of SIBs, as well as their excellent performance at cold temperature (Liu et al., 2019; Rudola et al., 2021b). Recent studies also projected that SIBs could cost 10–30 % less than LIBs, indicating them a more affordable energy storage option, especially in developing regions (Abraham, 2020; IEA, 2023; Rudola et al., 2023). Given the fact that sodium ions (Na+) has larger atomic radius than lithium ions (Li+), the volumetric energy density (Wh/L) of SIBs are intrinsically lower than that of most types of LIBs. Based on predictions and early-stage research results from academia and industry, SIBs could reach comparable specific energy (Wh/kg) to lithium iron phosphate (LFP) batteries (Abraham, 2020; Rudola et al., 2021a). Therefore, SIBs are suitable for applications that do not require high energy density, such as stationary storage and short or medium range electric vehicles (EVs) (Rudola et al., 2023).

Several life cycle assessment (LCA) studies have evaluated the environmental impacts of SIBs (Peters et al., 2016, 2021; Schneider et al., 2019). Additionally, some studies have specifically focused on anode or cathode materials of SIBs (Baumann et al., 2022; Peters et al., 2020; Rey et al., 2022). However, there is a lack of research considering future climate impacts of SIBs. As society undergoes a swift transition towards decarbonization, especially in high energy-intensive sectors, it is expected that the environmental impact of battery cells will be reduced due to the decarbonization of these upstream production processes. Additionally, such transition may alter or uncover environmental hotspots. Therefore, this study aims to perform a prospective life cycle assessment (pLCA) to explore the climate impacts of three promising SIBs produced in 2030, 2040, and 2050, with 2020 as the base year to compare.

2. Materials and method

2.1. Overall approach

Prospective life cycle assessment was conducted to assess future climate impacts of three sodium-ion batteries (SIBs), and to compare with two lithium-ion batteries (LIBs). The functional unit (FU) is 1 kWh of energy delivered over the battery’s lifetime. This study only considers climate impacts because the integrated assessment model (IAM) used to explore future scenarios focuses on changes in greenhouse gas (GHG) emissions. Given the recent emergence of SIBs in the market, high uncertainty exists in their end-of-life phase, and therefore it was not included in this study. The system boundary includes raw material extraction, transportation, production of precursors, production of battery components, battery manufacturing processes, and use phase by considering the depth of discharge (DoD), lifetime (in cycles) and roundtrip efficiency. The climate impacts associated to battery production is therefore calculated as the following equation:

$$\text{Climate impacts per FU} = \frac{\sum i * IS_i}{specific\ energy \times DoD \times lifetime \times roundtrip\ effciency} \quad (1)$$

i refers to the amount of battery components and manufacturing energy needed for producing 1 kg of battery, IS_i refers to the impact scores (kg CO_2-eq) for producing each unit of battery component and energy. Climate change impacts were computed using IPCC 2013 (100 year time frame) GWP characterization factors. The production of the battery cells was assumed to take place in Europe.

2.2. Life cycle inventory

2.2.1. Battery technologies

Three promising SIBs, with a technology readiness level of 9, were considered in this study based on market and research preference: layered oxide $Na_{1.1}(Ni_{0.3}Mn_{0.5}Mg_{0.05}Ti_{0.05})O_2$ (NMMT), vanadium-based polyanionic $Na_3V_2(PO_4)_2F_3$ (NVPF), and Prussian blue analogues $Na_2FeFe(CN)_6$ (NaPBA). Companies like Faradion Limited, Tiamat, Altris AB, etc., are working on mass-producing the above mentioned battery types (Rudola et al., 2021a; Tapia-Ruiz et al., 2021; Usiskin et al., 2021). To gain a better understanding of the environmental performance of SIBs, two LIBs: LFP and NMC 811 were included for comparison. LFP battery chemistry was selected because SIBs are expected to be used in similar applications as LFP batteries are presently deployed (Abraham, 2020). NMC811 battery chemistry was selected because nickel-rich layered oxide batteries are expected to be dominating the future market to address the urgent demand for energy storage (Kim et al., 2019; Wenjun et al., 2020).

To facilitate a fair comparison, all batteries were designed as the classic 21,700 format, which features a cylindrical shape with a diameter of 21 mm and a height of 70 mm (Fig.1). Instead of estimating or collecting the percentage of battery components and specific energy values from different literature sources, a battery dimensioning model was established for calculating the amount of each battery material required for studied battery chemistries as well as the corresponding specific energy, which increases the comparability analysis among batteries. The cylindrical cells were manufactured by rolling the battery layers into a cylindrical roll. It was assumed that the thickness of the cylindrical roll (which consists of current collectors, double-side coated electrode, and separators) was uniform at all points, and wound through an Archimedean spiral curve. The amount of each battery component was calculated based on Archimedean spiral curve functions, in combination with thickness of layers or mass loading of electrode active material, physical properties of materials (e.g. density, porosity), and inner volume of battery cell (Waldmann et al., 2020). The above-mentioned parameters use data collected from battery literatures, detailed equations and assumptions can be found in supplementary materials (SM 1 and 2). The cell capacity (mAh), specific energy

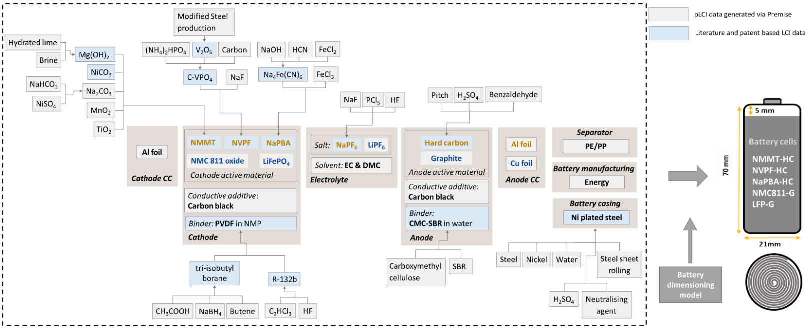

Fig. 1. Materials and energy required for cell production and their data source. Materials and energy within the shadow rectangles are directly used in battery manufacturing, others are upstream materials. Boxes featuring bold yellow words refer to materials only used in SIBs, boxes with bold blue words refer to materials only used in LIBs, boxes with words in bold black refers to materials used in both SIB and LIB. Italic words indicates the names of the battery components. CC refers to current collector; PVDF refers to polyvinylidene fluoride; NMP refers to N-methylpyrrolidone; EC refers to ethylene carbonate; DMC refers to dimethyl carbonate; PE/PP refers to polyethylene/polypropylene membrane.

Table 1
Composition (wt-%) of studied battery cells. HC refers to hard carbon. G refers to graphite. CMC refers to carboxymethyl cellulose. SBR refers to styrene butadiene rubber, super C65 is a high performance conductive carbon black powder.

		NMMT//HC	NVPF//HC	NaPBA // HC	NMC811//G	LFP//G
Anode	Anode active material	23.2 % (HC)	19.2 % (HC)	18.8 % (HC)	20.8 % (G)	17.6 % (G)
	Super C65	0.8 %	0.6 %	0.6 %	0.4 %	–
	CMC-SBR	1.3 %	1 %	1 %	0.4 %	0.4 %
Cathode	Cathode active material	31.8 % (NMMT)	35.5 % (NVPF)	29.3 % (NaPBA)	34.0 % (NMC811)	36.8 % (LFP)
	Super C65	0.7 %	0.7 %	0.6 %	0.7 %	0.8 %
	PVDF	0.7 %	0.7 %	0.6 %	0.7 %	0.8 %
Current Collector	Al foil	8.6 %	7.2 %	7.9 %	13.5 %	3.3 %
	Cu foil	–	–	–	4.1 %	11 %
Electrolyte		16.5 % ($NaPF_6$)	17.6 % ($NaPF_6$)	20.8 % ($NaPF_6$)	13.5 % ($LiPF_6$)	14.3 % ($LiPF_6$)
Separator	PE/PP	1.4 %	1.2 %	1.3 %	1.4 %	1.2 %
Cell container	Steel sheet	15.2 %	16.1 %	19 %	10.5 %	13.9 %
Total weight		56.2 g	53.1 g	45 g	64.2 g	61.4 g

(Wh/kg), and energy density (Wh/L) of the battery cells was then calculated based on cathode active material capacity (mAh/g), the amount of cathode active material, average voltage of the cell, and the total weight and volume of battery cell (Kevin et al., 2022) (detailed calculation can be found in SM 1 and 2). As a result, NMMT and NaPBA showed comparative specific energies as LIBs, which aligns with the perspective given in Peters et al. (2016). Battery dimensioning model can be found in SM 2. The battery composition results are presented in Table 1.

2.2.2. Data sources

Fig. 1 illustrates the battery materials used in the studied batteries and the life cycle inventory (LCI) data sources. Inventory data for material production and emissions from latest literature and Premise (Sacchi et al., 2022) generated prospective LCI (pLCI) databases was used directly or with modification for battery materials. Further details regarding the generation processes of the pLCI database can be found in Section 2.3.

For cathode active materials, production process and emission data for NMMT and NaPBA were extracted from previous studies (Peters et al., 2016, 2021), while LCI data of NVPF was established using production method described in Bianchini et al. (2014), further details can be read in SM 1. V_2O_5, a precursor in NVPF production process, was modeled as a by-product in primary steel production. The LCI of the steel production process was allocated to the products based on their economic values, a widely adopted allocation method in the ecoinvent database. As a result, 2 wt.% V_2O_5 in the overall products accounted for 36.7 wt.% of the LCI due to its high economic value. The V_2O_5 inventory comprised of 89 % production in China (Chen et al., 2015) and 11 % production in South Africa (Weber et al., 2018), reflecting reorganized market share data from USGS (2022). The production process description and detailed inventory can be found in SM 1 and 2.

As for anode active material, the most commonly used anode material for SIBs: hard carbon, was used. It was modeled using petroleum pitch as precursor due to its high carbon residue and low cost (Xie et al., 2010). The electrolyte is 1 M solution of sodium hexafluorophosphate ($NaPF_6$) in a mixture solvent of ethylene carbonate (EC) and dimethyl carbonate (DMC) (1:1). $NaPF_6$ was modeled based on inventory data in Peters et al. (2016). As sodium does not alloy with aluminum at the anode, aluminum foil was used as the current collector for both electrode. It was assumed that the separator of SIBs is identical to that of LIBs, polyethylene/polypropylene (PE/PP) membrane was therefore used in the study. LCI for current collector and separator was from pLCI

Table 2
Energy requirement for battery manufacturing (modified based on Yuan et al. (2017)).

Battery manufacturing process	Energy consumption
Electrode mixing and coating, calendaring, notching	3.8 kWh/ kg electrode
Electrodes drying and solvent recycling	10.6 kWh/ kg recovered solvent
Electrolyte filling	11.2 kWh/kg electrode
Dry room operation	4.1 kWh/kg electrode

databases. Finally, battery casing is nickel-plated steel sheet, and the production data was from Chordia et al. (2021). When energy consumption data in material production processes not available, it was estimated by methods presented in Piccinno et al. (2016). Detailed inventory generation processes can be found in SM 1 and 2.

Energy needed for battery manufacturing was estimated based on industrial data for manufacturing LMO-graphite battery. Inventory data provided by Yuan et al. (2017) were reorganized and summarized as parameters presented in Table 2. The considered manufacturing processes comprise of electrodes manufacturing (including electrode mixing and coating, calendaring, and notching), electrode drying and solvent recycling; electrolyte filling; and dry room operation. Calculation details can be found in SM 1 and 2. This study assumed electricity to be the only energy source in battery manufacturing processes, an assumption made to align with the reality in giga factories (Kurland, 2020). The European electricity mixture was used. Note that both battery manufacturing processes and battery composition were assumed to remain the same in the future years.

2.3. Scenario development

To assess the future climate impacts of studied batteries, potential future changes in the upstream systems were considered based on two background scenarios: SSP2-NDC and SSP2-PkBudg500. SSP2 corresponds to the Shared Socioeconomic Pathway narrative 2, representing a continuation of historical development trends in social, economy, and technology aspects (Riahi et al., 2017). NDCs and PkBudg500 represent two climate targets: national determined contributions and the 1.5 °C Paris Agreement. Following SSP2-NDC and SSP2-PkBudg500 scenarios, the increase of global mean surface temperature can be limited to 2.5 °C and 1.5 °C by 2100 respectively. For simplicity, we refer to these as the "2.5 °C" and "1.5 °C" scenarios in subsequent paragraphs. Another two foreground scenarios captured possible changes in battery performance: “Baseline performance” and “Optimal performance” scenarios. Consequently, this study included four combinations of foreground and background scenarios to explore future changes within the battery system: 2.5 °C - Baseline performance, 1.5 °C - Baseline performance, 2.5 °C - Optimal performance, and 1.5 °C - Optimal performance (Table 3).

Based on the narrative of these 2.5 °C and 1.5 °C scenarios, integrated assessment model (IAM) REMIND was used to model potential transformation changes in various sectors and regions (Baumstark et al., 2021), such as future electricity source, fuel generation technologies, improvements in production and process efficiency for energy intensive processes and materials, the implementation of Carbon Capture and Storage (CCS) technology, and shifts in material and energy market share. Next, such transformation changes were used to modify corresponding unit processes in ecoinvent database 3.8 using the Python package Premise (Sacchi et al., 2022), to generate pLCI databases (Premise: a Python package to integrate IAMs outputs with LCI databases). These pLCI databases were exported in a superstructure format (Steubing and de Koning, 2021), which was then used to model the total greenhouse gas emission of the battery system in the Activity Browser software (Steubing et al., 2020).

It is important to note that industry-specific electricity, such as those used by the aluminum, cobalt, and copper industries, were assumed to use the same production processes as current situation. Such assumption is based on the fact that these industries primarily rely on electricity generated by internal power plants rather than the general power grid. In addition, fossil fuel power plants such as coal plants have a long lifetime (typically over 50 years) (Cui et al., 2019). Hence, the private sector would likely economically favor the continued use of existing infrastructure until its designated end of life. Additional details regarding the REMIND model outputs and modifications made in the ecoinvent database can be found in Sacchi et al. (2023).

Table 3
Scenario combinations.

Scenario names	Background scenarios	Battery performance scenarios
2.5 ℃ - Baseline	SSP2-NDC	Baseline performance
1.5 ℃ - Baseline	SSP2-PkBudg500	Baseline performance
2.5 ℃ - Optimal	SSP2-NDC	Optimal performance
1.5 ℃ - Optimal	SSP2-PkBudg500	Optimal performance

The Baseline performance scenario refers to the performance that studied batteries could most likely achieve based on current research. Considering the early development of SIBs and the rapid advancements in the field (Tarascon, 2020), the battery performance may develop faster than expected. Therefore, the best-reported or projected data from battery studies were employed to represent the optimal battery performance. Both battery performance scenarios remain consistent in future years. The technical details of the studied batteries under these two scenarios are presented in Table 4.

The cathode capacity (mAh/g) for each cathode active material in both battery performance scenarios was collected from previous battery studies, and detailed data source can be found in SM 2. Battery lifetime is a parameter characterized by significant uncertainty due to factors such as operation conditions, charging rate, and charging depth (Han et al., 2019). In this study, we define lifetime as the number of charge–discharge cycles a battery can undergo before reaching 80 % of its initial capacity, with 80 % discharge depth (Table 4). The baseline performance scenario assumed 4000 cycles for NMMT (Faradion, 2022) and NMC 811 (Peters et al., 2021), 5000 cycles for NVPF (Tiamat, 2022), and 7000 cycles for NaPBA and LFP (Peters et al., 2021) (Table 4). The optimal battery lifetime values were derived from the best-reported or projection values (Peters et al., 2021; Tapia-Ruiz et al., 2021; Xiao et al., 2023; Zhao et al., 2022). Roundtrip efficiency values were based on previous reported value (Peters et al., 2021; Tapia-Ruiz et al., 2021). Battery voltage and depth discharge remain consistent in both scenario.

3. Results and interpretation

This section is structured as follows: Section 3.1 uncovers the climate impact of batteries in the year 2020, Section 3.2 describes the climate impact of batteries produced in future years (2030, 2040, 2050), and Section 3.3 analyzes the relative contributions of battery materials and energy flows to the overall assessment.

3.1. Climate impacts in 2020

The variation observed in the climate impact results in 2020 was solely due to differences in battery performance scenarios (Fig. 2). Under the Baseline performance scenarios, the three SIBs demonstrated higher climate impacts compared to LFP (9.8 g CO_2-eq/FU). However, when compared to NMC 811 (18.9 g CO_2-eq/FU), NaPBA (11.8 g CO_2-eq/FU) and NMMT (16.6 g CO_2-eq/FU) displayed better performance in climate impacts. Notably, NVPF had the highest emissions at 22 g CO_2-eq/FU. The results are in line with those from Peters et al. (2021) for NMMT (17 g CO_2-eq/FU), and lower for NaPBA (16.7 g CO_2-eq/FU), due to updated cathode active material capacity data with higher value used in this study.

The disparities in GHG emissions across the studied battery chemistries primarily stem from variations in battery materials used as different material production require varying energy inputs and emit different types of amount of emissions, as well as battery performance-related factors, such as specific energy, cycle life, and roundtrip efficiency. Battery performance factors determines the amount of battery material required to achieve an equivalent FU (Eq. (1)). Consequently, battery chemistries with the optimal combination of these factors exhibit superior climate impact performance. For instance, NaPBA’s relatively low climate impacts can be attributed to the low GHG emissions associated with its battery materials, coupled with its extended lifetime, even though its specific energy is the lowest among all

Table 4
Technical details of studied 21,700-size battery cells under baseline and optimal scenario. HC refers to hard carbon, G refers to graphite.

Scenario		NMMT/HC	NVPF/HC	NaPBA/ HC	NMC 811 /G	LFP/G
Baseline performance	Voltage (V)	3.2	3.4	3	3.57	3.2
	Cathode specific capacity (mAh/g)	154	120	150	200	157
	Cell capacity (mAh)	2748	2268	1974	4361	3542
	Specific energy (Wh/kg)	157	145	132	243	185
	Volumetric energy density (Wh/L)	363	318	244	642	523
	Roundtrip efficiency	94 %	93 %	93 %	91 %	94 %
	Lifetime (cycles)	4000	5000	7000	4000	7000
	Discharge Depth	80 %	80 %	80 %	80 %	80 %
Optimal performance	Voltage (V)	3.2	3.4	3	3.57	3.2
	Cathode specific capacity (mAh/g)	215	138	160	213	165
	Cell capacity (mAh)	3837	2608	2106	4645	3729
	Specific energy (Wh/kg)	219	232	149	258	194
	Volumetric energy density (Wh/L)	506	366	261	684	551
	Roundtrip efficiency	95 %	97 %	97 %	95 %	95 %
	Lifetime (cycles)	8000	15,000	15,000	9000	10,500
	Discharge Depth	80 %	80 %	80 %	80 %	80 %

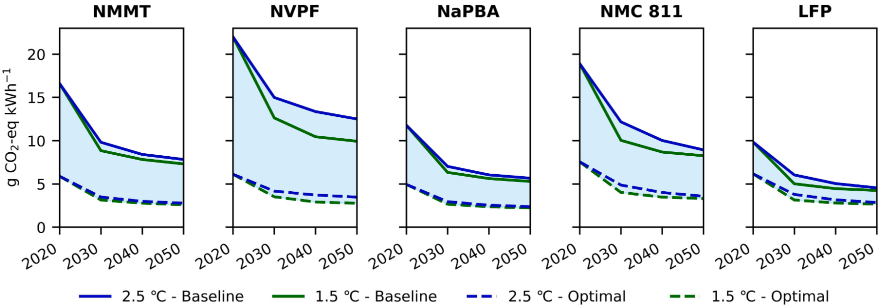

Fig. 2. Climate impacts results of studied batteries at different years, under four scenarios. Results are expressed per kWh of energy delivered along lifetime. The shaded blue area illustrates the disparity in climate impacts resulting from baseline and optimal performance scenarios.

investigated batteries. While the high climate impacts of NVPF can largely be attributed to the high GHG emissions embodied in the precursor material V_2O_5, as well as the inferior specific energy and cycle life of NVPF.

Applying optimal performance substantially reduced the climate impacts of the studied batteries, resulting in reductions of 65 %, 72 %, 58 %, 60 %, and 37 % for NMMT, NVPF, NaPBA, NMC 811, and LFP, respectively. Consequently, the three SIBs exhibited lower climate impacts than LIBs under Optimal performance scenarios.

3.2. Climate impacts in 2030, 2040, 2050

The total climate impacts for each battery chemistry decreased over time across all four scenarios (Fig. 2). It is important to note that these reductions were primarily driven by the implementation of 1.5 °C and 2.5 °C scenarios, as battery performance was assumed to remain consistent over time. When comparing the production of SIBs in 2050 to that of 2020, the 2.5℃ scenarios exhibited a reduction in climate impacts ranging from 43 % to 54 %, while the 1.5 °C scenarios demonstrated a slightly greater reduction of 55–57 % for studied SIB chemistries. As a result, the GHG emissions for three SIBs (NMMT, NVPF, NaPBA) and two LIBs (NMC 811 and LFP) at year 2050 are: 2.6–7.8 g CO_2-eq/FU, 2.8–12.5 g CO_2-eq/FU, 2.2–5.7 g CO_2-eq/FU, 3.3–8.9 g CO_2-eq/FU, 2.7–4.5 g CO_2-eq/FU. This trend is consistent with a recent study by Xu et al. (2022), although they only focused on future climate impacts for LIBs.

These reductions in climate impacts were predominantly attributable to decarbonization efforts within the energy sectors. The REMIND model projected a remarkable increase in the share of renewable resources (e.g., wind, solar, hydropower) in European electricity generation, rising from 39 % in 2020 to approximately 97–98 % in the 2.5 °C and 1.5 °C scenarios, respectively, by 2050. Consequently, the climate impacts of the European electricity mixture (at medium voltage) dropped from 310 g CO_2-eq/kWh in 2020 to 13.9–16.3 g CO_2-eq/kWh in 2050. In addition, the implementation of carbon capture and storage (CCS) technologies in the industrial power and heat generation processes also plays a significant role.

Furthermore, decarbonization strategies in the steel sector, such as improved energy efficiency, the implementation of CCS, and increased recycling and reusing of steel, played a significant role, particularly for NVPF. The GHG emissions of NVPF can be primarily attributed to the production of its precursor material V_2O_5, which was modeled as a co-product in steel production. Therefore, the 1.5 °C scenarios, with more stringent decarbonization strategies in the steel sector, lead to greater reductions in the climate impacts of NVPF overtime. For example, CCS is implemented in the steel sector under the 1.5 °C scenario but not in the 2.5 °C scenario. This explains the larger discrepancy in climate impact reduction for NVPF between the 2.5 °C and 1.5 °C scenarios compared to other battery chemistries.

3.3. Contribution analysis

Fig. 3 illustrated the contribution analysis under 2.5 °C and 1.5 °C scenarios. Total climate impacts were divided into emissions associated with the production of battery components (including cathode active material, anode active material, current collectors for both electrodes,

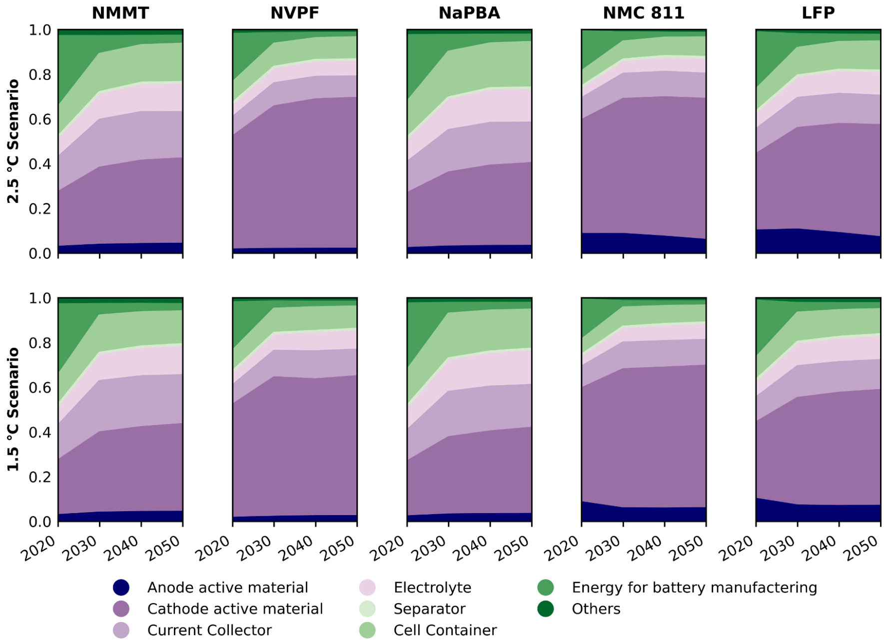

Fig. 3. Relative contributions to overall climate impacts from battery materials and energy use.

electrolyte, and cell container), energy used in battery manufacturing processes, and others (e.g. binders, conductive active material, etc.). Similar contribution results were obtained from both scenarios. It is worth mentioning that battery performance scenarios solely affect the overall climate impacts of batteries and do not impact the relative contributions of material and energy flows.

Cathode active materials were clearly key contributors in all investigated batteries, accounting for a relative contribution of 24–39 % for NMMT, 51–67 % for NVPF, 25–39 % for NaPBA, 51–64 % for NMC 811, and 34–52 % for LFP, regardless of the production year and applied scenarios. The relative contribution of cathode for NMMT and NaPBA is lower than that of LIBs, while the relative contribution of NVPF is higher than that of LIBs. The significant contribution of cathode active materials stemmed from mineral mining and processing steps (e.g., cobalt, nickel, vanadium oxide), high-emission production processes such as hydrogen cyanide production, and the substantial proportion of cathode active material in the battery cell by weight (Table 1). The relatively high contribution from cathode active material of NVPF is primarily associated with the production of precursor material V_2O_5. As described earlier, V_2O_5 is modeled as a by-product of primary steel production, a highly energy-intensive process. The economic allocation choice results in V_2O_5 with 2 wt.% of the overall products accounted for 36.7 % of the emissions due to its high economic value. The relatively high contribution from cathode active material in NMC 811 can be attributed to the production of precursor materials: cobalt sulfate and nickel sulfate, both related to cobalt production. Nickel sulfate was modeled as a co-product in the cobalt production processes. Nickel sulfate was also a raw material used in the production of cathode active material for NMMT, but 66 % less nickel sulfate is consumed in producing per kg of cathode active material in NMMT compared to that used in producing per kg of cathode active material in NMC 811.

Energy consumption during the battery manufacturing process emerged as another notable contributor to total emissions for the three studied SIBs at 2020, accounting for 18–32 % of total emissions. This substantial energy consumption in battery manufacturing processes can be primarily attributed to operations such as drying and solvent recovery (NMP) of the binder, dry room operation, and electrolyte filling. The finding is consistent with previous studies highlighting battery manufacturing as a significant source of GHG emissions (Peters et al., 2021; Schneider et al., 2019).

Additionally, the production of current collector (9–16 %), cell container (7–16 %), and electrolyte (5–10 %) are other important contributors to total GHG emissions of studied SIB chemistries at 2020. These emissions arise from manufacturing processes involving producing aluminum foil (current collector), and steel (cell container material). On the other hand, the production of the anode active material (1–3 %), namely hard carbon, made a minor contribution to the overall climate impacts in SIBs in 2020, despite accounting for 19–23 wt-% of the battery cell. Similar trends were also observed in Peters et al. (2021). In contrast, the anode active material in LIBs (graphite) contributed 8–10 % to total emissions in 2020, primarily due to the higher manufacturing temperature required for graphite than for hard carbon production.

From 2020 to 2050, significant contribution reductions from the battery manufacturing stage can be observed, which is due to the decarbonization in European electricity mixture. The decreased GHG emissions from the battery manufacturing process contributed to up to 66 % of the total reduction in climate impacts of investigated batteries. Consequently, the GHG emissions from the battery manufacturing process account for only 2–4 % of the total impacts in both scenarios by 2050. In contrast, the relative contribution from other material flows are likely to increase over time.

3.4. Sensitivity analysis

Notably, the choice of allocation methods can significantly influence the climate impacts of V_2O_5 (He et al., 2020), thus affecting the total

GHG emissions of the NVPF battery. He et al. (2020) highlighted the influence of allocation method on the environmental impacts of V_2O_5, when modeling it as a by-product of steel production. In this sensitivity analysis, we changed the allocation method used in production of V_2O_5 and crude steel from economic allocation to mass-based allocation. The sensitivity analysis results reveals a significant reduction of 40 % in the total climate impacts of NVPF battery, resulting in a similar environmental impacts as NaPBA (11.7 CO_2-eq/FU) in 2020.

4. Discussion

This study for the first time assessed the future climate impacts of SIBs while considering potential changes in both the foreground and upstream aspects of the battery system. Lai et al. (2023) conducted an LCA on various sodium battery technologies using future Chinese electricity mixtures in the battery manufacturing processes, without considering potential future changes in the background system. This likely explains the significant disparity in future GHG emission results, which were up to five times higher than our findings when converted to the same FU.

The results underscore the critical importance of optimizing battery performance, a measure that can mitigate more climate impacts per FU than the decarbonization of energy-intensive sectors within the upstream system. This aligns with prior research emphasizing the significance of specific energy and battery lifetime in environmental impacts (Peters et al., 2017; Schneider et al., 2019). This insight could guide future research directions aimed at fostering the sustainable development of batteries. For instance, the scenario results suggested that enhancing the specific capacity (mAh/g) of the electrode active material could reduce the climate impacts of the cell. Additionally, modifying cell dimensions can also affect the climate impacts by influencing the specific energy of the cell.

Furthermore, the results highlight the SIBs' potential to either outperform or at least match LIBs in terms of climate impact, with optimization. This speaks in favor of supporting the further development of SIBs. Despite this potential, EU funding for SIB research has been minimal, accounting for only 2.5 % of public funding in battery research from 2014 to 2021 (Bielewski et al., 2022). SIBs offer a cost-effective alternative for stationary and vehicle applications, especially in developing regions and sectors prioritizing affordability, such as buses and trucks. Notably, over 50 % of truck consumers rely on leasing or loans for their purchases (IEA, 2023). Therefore, increased investment in SIB research holds the key to increasing its market penetration significantly and enhancing its climate impact performance.

Increasing the share of renewable energy in the power grid and steel industries and implementing CCS are also important for reducing GHG emissions in battery production. Achieving this requires concerted efforts not only from battery manufacturers but also from industries involved in the entire battery production chain, including electricity, heat and power, steel, and others. Future battery or battery component factories could consider locating near clean energy sources like hydropower, wind, or solar energy to further mitigate emissions.

An advantage of SIBs is their reduced reliance on critical materials such as cobalt and lithium, which were not assessed in this study. We conducted rough calculation based on scenarios presented in Xu et al. (2020) and the Electric Vehicles (EVs) development trend outlined in IEA (2023). Assuming 100 % market penetration of EVs by 2050 and a 60 % market share of LFP chemistry in EVs between 2030 and 2050, if SIBs could replace LFP entirely, the lithium demand could be reduced as much as 16.4 Mt by 2050. This equals to more than 50 % of current low-cost lithium resources (Greim et al., 2020). However, it is important to note that substituting LIBs with SIBs may increase demand for other materials like nickel, manganese, and vanadium.

There are other perspectives that have not been considered in this study. First, our focus was solely on climate impacts. This is because current scenarios and IAMs have detailed representations of narratives and sectors relevant to climate impacts, but do not have a specific focus on other environmental impact categories (Steubing et al., 2023). Future research should extend its scope to consider other environmental impact categories for a more comprehensive understanding and to avoid potential environmental burden shifting. To achieve this, a more comprehensive pLCI database need to be developed by including the future changes in sectors and environmental interventions related to other impact categories in IAMs (Steubing et al., 2023). Second, this study assessed battery chemistries at the cell level. In various applications, batteries are often used in modules and packs, with additional components like battery management systems and packages. According to Peters and Weil (2018), the average climate impacts for these additional battery components are approximately 2.2 $kgCO_2$-eq/kg battery. This suggests that the climate impacts of batteries at the module /pack are likely to favor battery chemistries with an optimal combination of performance (e.g. higher specific energy, longer cycle life). This is due to the correlation between higher performance and the need for fewer batteries, thereby resulting in lower greenhouse gas emissions. The environmental performance at module/pack level also depends on the specific design considerations, which could be explored in the future research. Third, we did not consider advancements in battery manufacturing method, which could lead to more efficient processes. However, our results indicate a relatively minor contribution from battery manufacturing processes when clean electricity is used. Moreover, end-of-life (EoL) stage of SIBs was not considered, as the primary focus was on battery production. EoL options, such as repurposing batteries for other applications or recycling raw materials, could mitigate environmental impacts over the battery's lifetime. While repurposing may not affect the relative environmental performance order among studied batteries, recycling battery raw materials may favor battery chemistries using minerals with high GHG emissions, such as NVPF and NMC 811. However, the economic viability of recycling SIBs remains uncertain due to their lower economic value compared to LIBs. What's more, this study used fossil-based precursors for hard carbon (anode active material) in the model due to its low cost and high carbon residue. While extensive research has explored the use of biomass as a precursor to produce hard carbon, previous studies have highlighted that SIBs with biomass-based hard carbon anode generally show higher climate impacts compared to fossil-based alternatives (Peters et al., 2019). Among various organic precursors, organic waste like apple pomace demonstrates favorable climate impact performance (Peters et al., 2019). However, addressing the challenge of ensuring consistency in organic flow and content is crucial to secure a robust supply chain. Last but not least, the rapid development of other promising battery technologies, like all-solid-state sodium ion batteries, requires future studies to assess their environmental performance, which falls outside the scope of this study.

5. Conclusion

Based on the functional unit of 1 kWh of energy delivered over lifetime, the results show that sodium-ion batteries (SIBs) have the potential to perform equal or better in climate impacts than lithium-ion batteries. Achieving this potential requires efforts and increased investment in SIBs research and development by battery researchers. The climate impacts of SIBs exhibited a reduction of 43–57 % by 2050 compared to their 2020 levels. This reduction is primarily attributed to the increasing penetration of renewable energy sources in the grid electricity mix and substantial decarbonization efforts undertaken within the steel sector. The relative contribution of battery manufacturing processes to the total emission decrease significantly over time, while the relative contribution of cathode active material increase over time. Existing battery industries can prioritize the use of clean energy sources for manufacturing batteries to mitigate their climate impacts. Future battery facilities may consider strategic locations close to regions where clean energy is abundantly produced.

Moreover, sensitivity analyses underscore the impact of allocation methods used in precursor material of the NVPF's cathode active material on results.

CRediT authorship contribution statement

Shan Zhang: Conceptualization, Methodology, Software, Formal analysis, Investigation, Writing – original draft, Writing – review & editing, Visualization. **Bernhard Steubing:** Methodology, Writing – review & editing. **Hanna Karlsson Potter:** Supervision, Writing – review & editing. **Per-Anders Hansson:** Supervision, Funding acquisition. **Åke Nordberg:** Supervision, Writing – review & editing.

Declaration of Competing Interest

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.

Data availability

Data will be made available on request.

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Supplementary materials

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.resconrec.2023.107362.

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Population growth, economic development, and electrification are increasing demand for advanced batteries, driving the development of next-generation battery technologies. This thesis assesses the environmental impacts of all-organic, all-solid-state, and sodium-ion batteries using life cycle assessment (LCA), and prospective LCA. The results provide important insights that can inform the development of more environmentally friendly battery technologies.

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