



## 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 <sub>4</sub> Ti <sub>5</sub> O <sub>12</sub> /Lithium Titanate Oxide
PDMS	Polydimethylsiloxane
Pd(PPh <sub>3</sub> ) <sub>4</sub>	Tetrakis(triphenylphosphine)palladium(0)
CHCl <sub>3</sub>	Trichloromethane
CNT	Carbon nanotube
EDOT	3,4-Ethylenedioxythiophene
ProDOT	3,4-propylenedioxythiophene
pEP(QH <sub>2</sub> )E	p refers to polymerized, E to 3,4-ethylenedioxythiophene, P to 3,4-propylenedioxythiophene, QH <sub>2</sub> 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 <sub>f</sub>	A future point in time
T <sub>0</sub>	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<sub>f</sub>) 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<sub>0</sub>) to T<sub>f</sub> (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<sub>0</sub> 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<sub>0</sub>) to industrial scale (T<sub>f</sub>) (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<sub>f</sub>). 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.

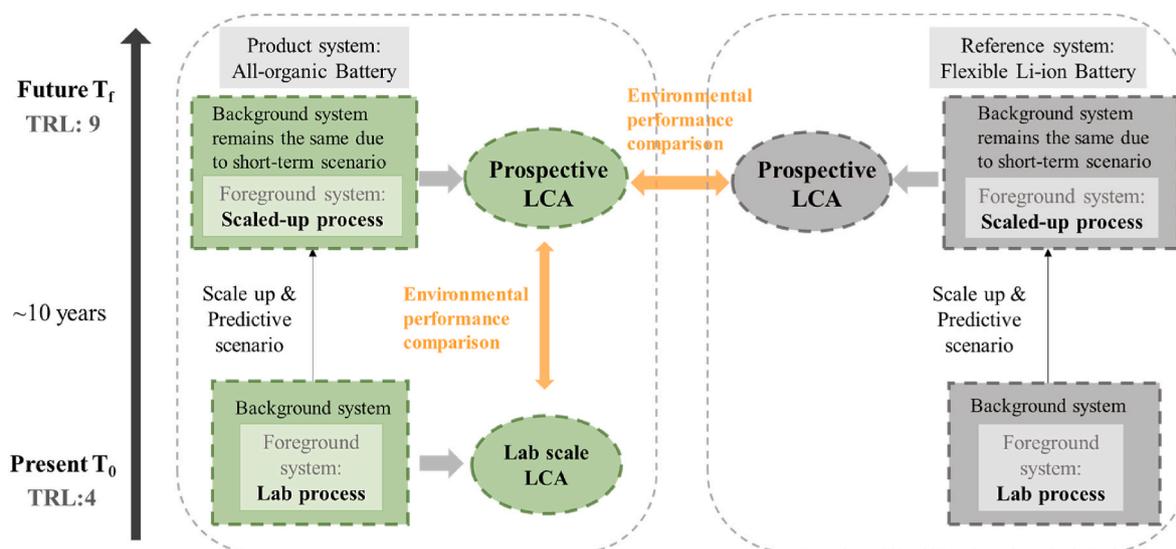
### 2.1. Goal and scope

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.

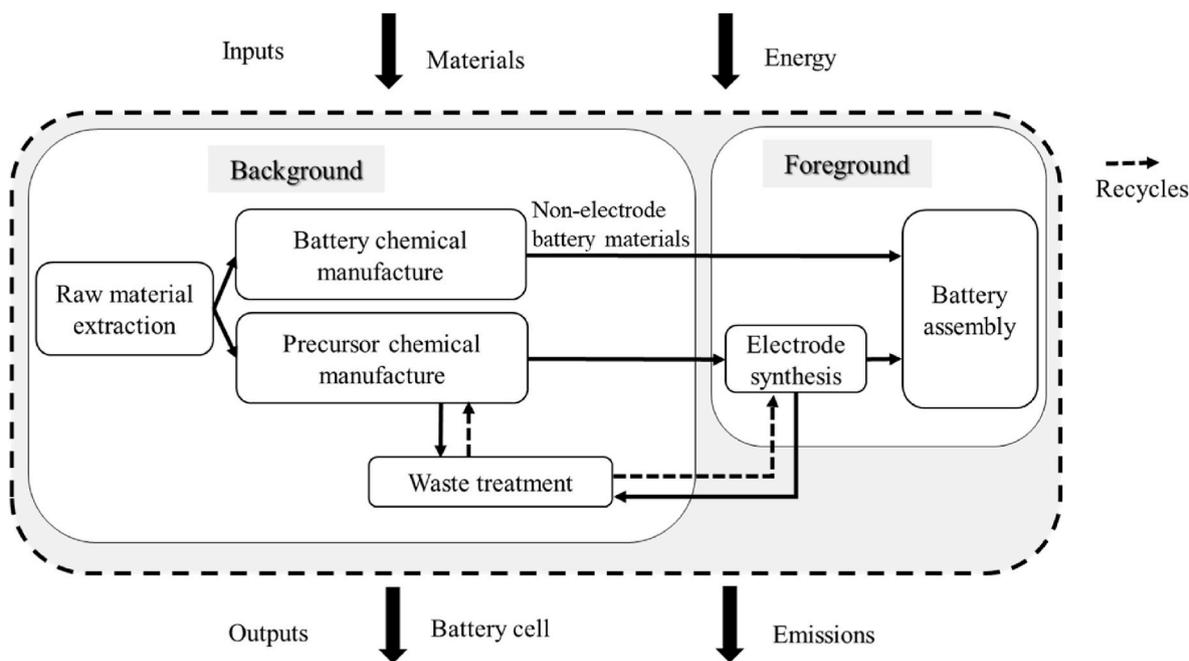
### 2.2. Life cycle inventory and data sources

#### 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<sub>2</sub>)E and pEP(NQ)E, with trimeric thiophene repeating units (EPE) as backbones and quinone-based pendant groups (QH<sub>2</sub> and NQ). The electrolyte is 0.5 M H<sub>2</sub>SO<sub>4</sub> (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<sub>0</sub>) at the bottom and future time (T<sub>f</sub>), 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<sub>4</sub>Ti<sub>5</sub>O<sub>12</sub> (LTO) and LiCoO<sub>2</sub> (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<sub>6</sub>-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

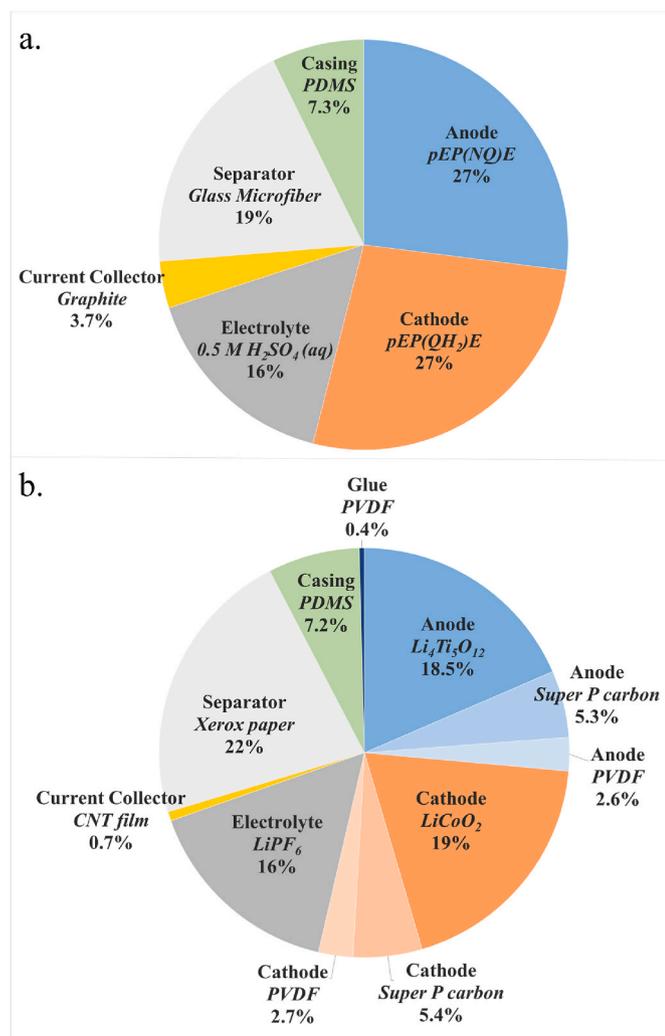


Fig. 3. Composition (wt-%) of the all-organic battery (a) and the Li-ion battery (b).

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<sub>3</sub>)<sub>4</sub> 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<sub>3</sub>)<sub>4</sub> 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<sub>3</sub>)<sub>4</sub> 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<sub>2</sub>-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<sub>3</sub>Cl/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<sub>2</sub>, 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<sub>2</sub> in other impact categories were minor (<1%).

Solvents were the dominant contributors (89%) to ozone depletion

potential (Fig. 4). Trichloromethane (CHCl<sub>3</sub>) were the most significant contributor, accounting for 74% of the total ozone depletion potential. Most of the CHCl<sub>3</sub> (>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<sub>3</sub> is due to carbon tetrachloride (CCl<sub>4</sub>) emissions during production of CHCl<sub>3</sub>. It has been shown that use of CHCl<sub>3</sub> 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 <sub>2</sub> -eq	22%	2%	9%	46%	15%	5%	1%
Ozone depletion	5.3 × 10 <sup>-5</sup> kg CFC-11-eq	26%	1%	20%	42%	0%	2%	9%
Human toxicity, non-cancer effects	1.7 × 10 <sup>-6</sup> CTUh	27%	2%	6%	48%	11%	3%	2%
Human toxicity, cancer effects	4.9 × 10 <sup>-7</sup> 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 <sup>2</sup> CTUe	27%	2%	6%	51%	11%	2%	1%
Mineral, fossil & renewable resource depletion	1 × 10 <sup>-3</sup> kg Sb-eq	35%	0%	1%	52%	11%	1%	0%

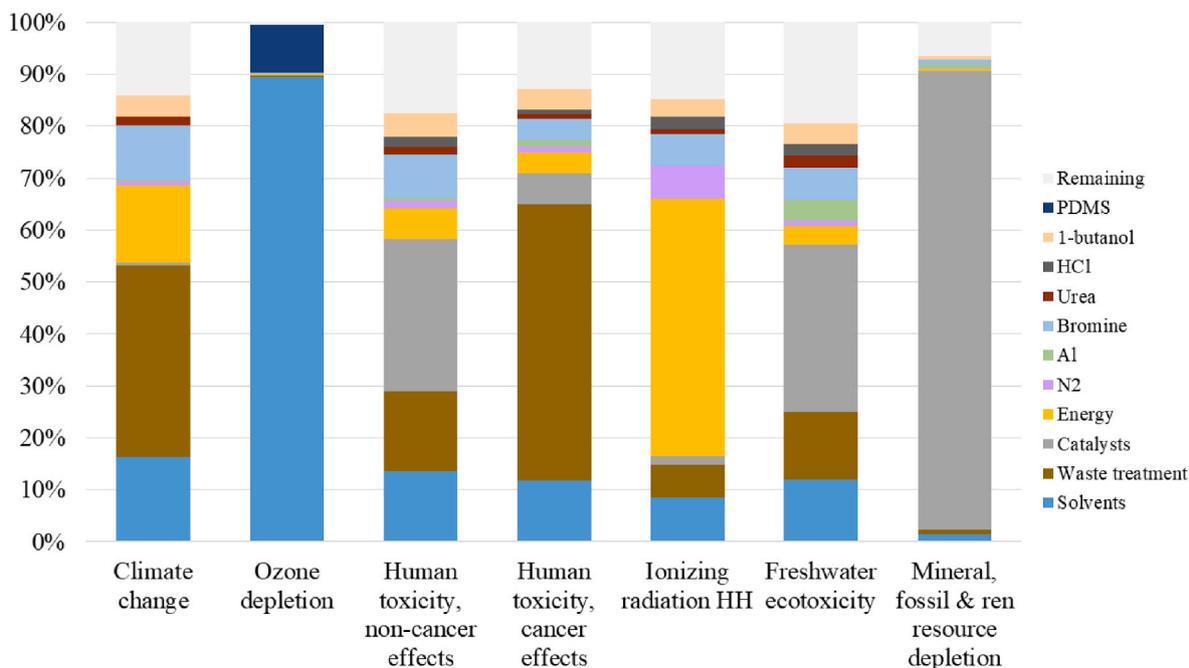


Fig. 4. Relative contribution of different process flows in industrial-scale production of organic batteries to the most significant impact categories.

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  $8.7 \times 10^7$  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

Table 3

Comparison of environmental performance of the flexible Li-ion battery and of all-organic batteries with different cycle lives (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

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).

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 over-estimates 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<sub>2</sub> with Cl<sub>2</sub>

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

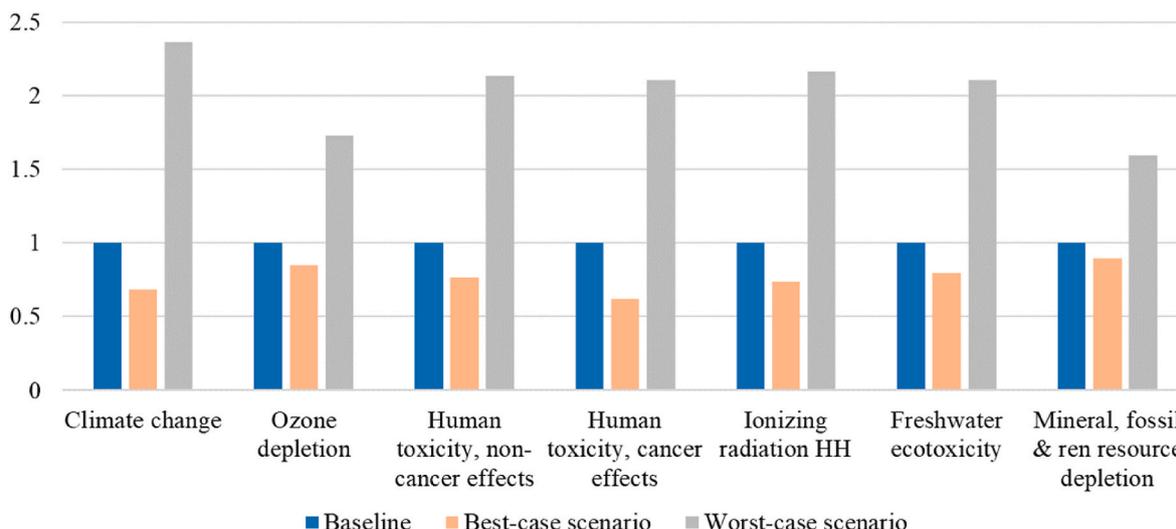


Fig. 5. Influence of scaling up parameters.

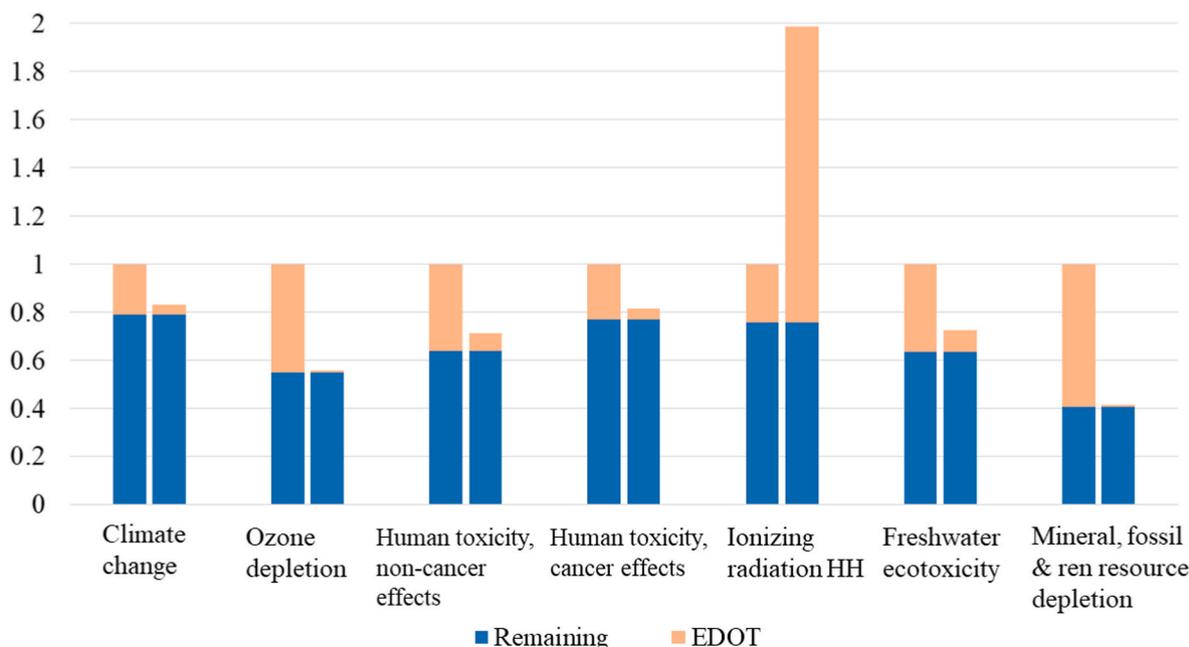


Fig. 6. Effect of changing 3,4-ethylenedioxythiophene (EDOT) production route on the environmental impact in significant impact categories assessed in this study. For each impact category, the left column refers to the baseline LCA result, while the right column refers to the LCA result after changing 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	Abiotic depletion method	1	29	7
Midpoint (2011)	Surplus ore potential method	1	18	4
ReCiPe 2016 (H) V1.04				

brominated aromatic hydrocarbons (Br<sub>2</sub>ProDOT-OH) used in production of the all-organic battery cells were assumed to be replaced with chlorinated aromatic hydrocarbons (Cl<sub>2</sub>ProDOT-OH) (Fig. S1). The results

showed that changing the raw material from Br<sub>2</sub> to Cl<sub>2</sub> 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

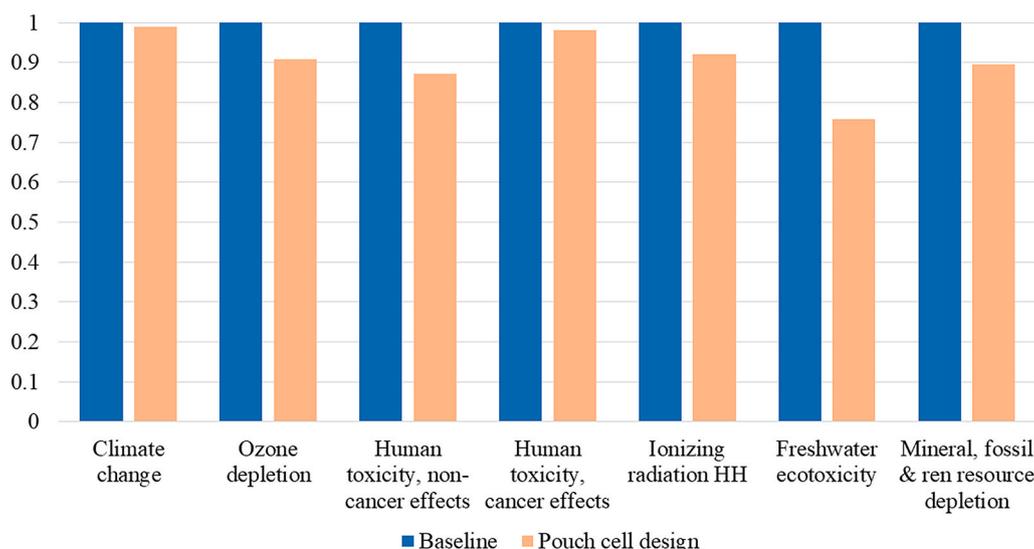


Fig. 7. Effect of changing battery design on the environmental impact in significant impact categories assessed in this study.

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<sub>2</sub>-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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