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ORIGINAL PAPER

Towards Sustainable Circularity? Prospective Life Cycle Assessment of Lithium-Ion Batteries with Bio-Based Materials

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Abstract

This prospective cradle-to-gate life cycle assessment evaluates lithium-ion battery pouch cells utilising novel bio-silica electrolytes and bio-silicon anodes and aims to integrate environmental sustainability and circularity considerations early in process development. Although the bio-silica and bio-silicon are sourced from barley husk bio-waste with minimal upstream burden, current processing routes are energy- and chemically intensive and generate substantial acid waste. Reliance on high-temperature treatments makes renewable electricity essential. Climate-change impact of cells utilising the novel materials falls from 13,200 kg CO_2-eq/kWh at lab-scale to 62 kg CO_2-eq/kWh when certain key parameters were optimised in an industrial scenario. Key levers for impact reduction include increasing active-material capacity, applying pre-lithiation, and optimising anode processing. However, even the best-case manufacturing energy demand (207 kWh/kWh cell) is around double that of conventional giga-factory production, underscoring the need for process innovation. From a circularity perspective, low material yields and high chemical intensity limit net environmental benefits, demonstrating that circular feedstocks do not inherently deliver sustainable outcomes. For developers, the results highlight the importance of more resource-efficient, higher-yield, and less energy-intensive routes to bio-silica and bio-silicon production, including feedstocks with higher silica content. For LCA practitioners, they emphasise challenges of scaling lab data and the scarcity of industrial benchmarks. Overall, bio-waste represents a potentially valuable feedstock for circular battery materials, although realising sustainable circularity depends on advances in processing efficiency and system-level optimisation.

Keywords Lithium-ion battery · Silicon · Bio-materials · Sustainability · Life cycle assessment · Circularity

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Extended author information available on the last page of the article

Introduction

Meeting decarbonisation targets requires large-scale energy storage and fast-response flexibility, with sector-specific needs. In the power sector, rechargeable batteries enable the integration of variable renewables, provide peak-load support, and enhance grid stability. In transport, electrification is a central decarbonisation strategy, relying on rechargeable batteries across hybrid, battery-electric, and fuel cell electric powertrains. Lithium-ion batteries (LIBs) have become the predominant rechargeable battery choice for both electrical energy storage [1] and transport electrification [2] due to favourable characteristics such as high energy and power density, excellent cyclability, and reliability [3].

Despite being the most mature and widely deployed energy storage technology, LIBs face several well-documented challenges, including the use of flammable organic liquid electrolytes and proximity to their theoretical limits in power and energy density [4]. With rapid growth in LIB production and use, sustainability has also become a critical issue [5, 6], which includes 1) relatively high environmental impacts associated with production, 2) use of raw materials defined as critical in the European Union, and 3) ethical concerns relating to mining and extraction. The challenges have sustained continued research into next-generation LIBs [7, 8], such as the development of silicon (Si) anodes with higher specific capacity than graphite as well as solid-state electrolytes. Another common thread is the use of bio-waste [9, 10] and industrial-waste [11, 12] as a resource, particularly for developing sustainable materials that can be used in batteries, including bio-Si production [13–15].

The use of bio-waste and industrial-waste streams is increasingly promoted within EU circular economy frameworks as a means to reduce reliance on virgin resources, improve resource efficiency, and divert materials from disposal pathways in line with the waste hierarchy [14–16]. By using these residual materials, potential reductions in life cycle environmental impacts exist [14], particularly if fossil-fuel derived materials are displaced. However, circularity does not always equate to environmental sustainability [17] with possible trade-offs entailing high material and energy needs for processing [13–15]. This underscores the need for life cycle assessment (LCA) to ensure net sustainability benefits.

Forward-looking comparison is required to identify early-stage technology options with genuine performance and sustainability advantages before large resources become sunk costs. However, this is particularly challenging given the emerging setting of technological developments, and the fact that much early research is explorative. Use of prospective LCA (pLCA) allows for assessments of emerging technologies and simulated production scale-up, and thereafter investigation of environmental impacts [18, 19]. Process and design optimisation, together with economies of scale, can lead to substantial improvements; for LIB manufacturing, energy demand has been shown to decrease by nearly two orders of magnitude when scaling from laboratory to industrial production [20]. Multiple prior studies have applied pLCA to emerging battery technology [21–25]. Examples of focus for post-lithium technologies include sodium-ion [26, 27] and magnesium [28] batteries, with use of bio-materials also discussed [26, 27].

Scenarios in pLCA are crucial to demonstrate potential improvements in the foreground and background of a technology and to account for associated uncertainties in future development [18, 29]. Recent developments in the pLCA field have made available various frameworks [29], life cycle inventory (LCI) data [30], and methods for upscaling processes (see e.g., [31] for a review). Nevertheless, scaleup remains challenging since refined data, specific assumptions and information can still be difficult to obtain [32].

In this study, we apply pLCA to an emerging next-generation bio-based LIB technology to assess environmental impacts and guide development in the most environmentally sustainable direction possible. The investigated technology contains innovations in both the anode and electrolyte (including use of bio-Si) with materials derived, to the extent possible, from bio-sourced precursors available in European countries. The technology is currently at lab-scale, with production limited to grams per batch and with data constrained to what is available from lab-scale development by researchers. This starting point illustrates the typical challenges associated with applying pLCA to emerging technologies, making the study relevant not only for technology developers and for assessing the environmental sustainability of bio-based materials, but also for LCA practitioners wanting to better understand the strengths and limitations of pLCA methodologies.

Circular Bio-Based Materials for Battery Production

The battery assessed in this study combines an anode containing mesoporous bio-Si derived from waste barley husks and carbon nanofibre (CNF) derived from nano-fibrillated cellulose (NFC), a *quasi*-solid-state electrolyte, and a cathode using commercially sourced LFP. The electrolyte incorporates bio-silica (SiO_2), obtained as an intermediate in the conversion of barley husks to bio-Si. Copper and aluminium current collectors are needed, but the battery design aims to reduce the weight of the copper current collector for the anode due to the use of CNF.

Several theoretical benefits are associated with this setup. Firstly, integrating bio-Si into anodes in LIB enhances energy density due to differences in theoretical specific capacity [33]. Secondly, the introduction of a *quasi*-solid-state electrolyte helps address many challenges linked to the use of organic liquid electrolytes, such as leakage and flammability. Finally, the sustainability profile can be improved by using bio-based materials, reducing copper demand, and avoiding upstream social and human-rights risks in cobalt supply chains. An overview of the concept and approach is depicted in Fig. 1.

The technology is currently at Technology Readiness Level (TRL) 2 with individual components already demonstrated in the laboratory within the project. The project end target was set to TRL 4 with a lab-scale pouch cell prototype assembled and at least some individual components of the battery showing industrial relevance. Secondary objectives in terms of key performance indicators (KPIs) were set for both the anode (anode capacity of 600 $mAh/g_{\text{active material}}$ and an optimal ratio of bio-Si to CNF), as well as the *quasi*-solid-state electrolyte. Since the CNF is amorphous carbon, we assume it has a maximum ~ 15% contribution to anode capacity. Note that the surface area of CNF is 231 m^2/g and the porosity is 48%.

Method

This study primarily aimed to assess the environmental performance of the developed battery cell at lab-scale (0.2 Ah pouch cell) and to explore strategies for optimising its development toward industrial maturity (TRL 9, 10 Ah pouch cell). We also focused on the bio-Si

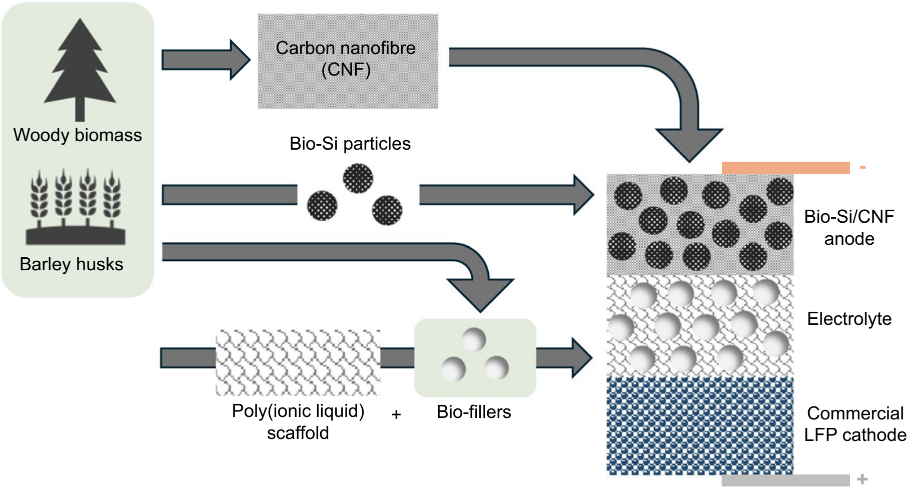

Fig. 1 The battery concept and approach. Bio-based materials are denoted with a light green background

material, since it underpins the cell concept. For this purpose, we carried out a prospective cradle-to-gate attributional LCA using explorative what-if scenarios to evaluate how different development routes affect future production impacts of the cell. Based on the findings, we discuss implications for future development. The assessment was carried out using process-based attributional modelling, applying the cut-off allocation approach.

The system boundaries included production stages starting with raw material extraction and ending with formation cycling (see Fig. 2 for a flowchart). In the flowchart, we distinguish between the foreground and background systems depending on which parts are under direct influence of the battery developers. The foreground system covers production

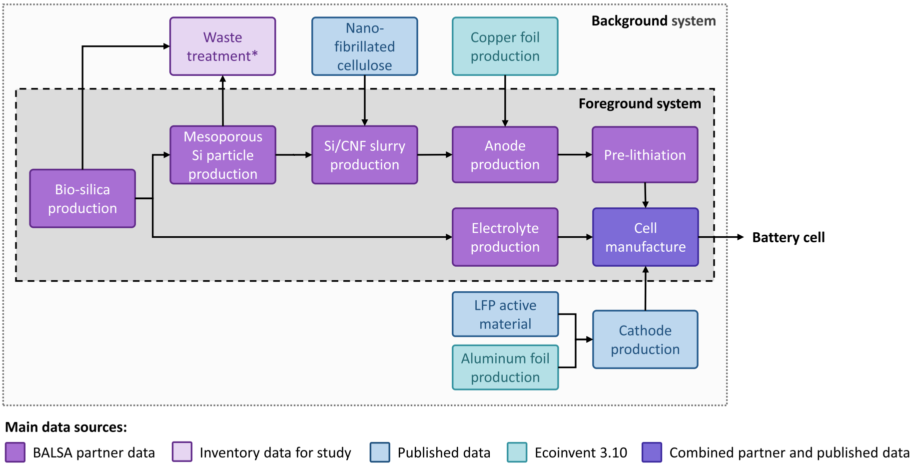

Fig. 2 Simplified flowchart showing system boundaries and main data sources. Pre-lithiation was an optional process. *While final disposal was treated as part of the background system, recovery processes were modelled explicitly within the foreground system

of the bio-SiO_2 precursor, mesoporous bio-Si particles, Si/CNF slurry, anode, pre-lithiation, electrolyte, and cathode, along with cell assembly and formation. Pre-lithiation is currently investigated mainly at lab- and pilot-scales as a way to mitigate initial lithium losses in high-capacity anodes, thereby enhancing energy density and cycle life [34]. It was not included in the lab-scale process but modelled as an optional extension in this prospective study. The background system covers upstream processes such as waste treatment (with recovery processes modelled in the foreground) and production of NFC, LFP active material, current collectors, and the complete cathode.

A European geographical system boundary was considered, involving development of European supply chains and production. As such, background data largely represent European averages, or global averages where European averages were unavailable. In terms of temporal system boundaries, we assumed that lab-scale production at TRL 4 occurs in 2025, while industrial production at TRL 9 would take place in 2040.

In line with the attributional approach taken in the study, co-production was dealt with through partitioning allocation—a process that splits co-production requirements proportionally according to a common property (e.g., mass, energy content, or value) using a partitioning coefficient with a value between zero and one [35].

A functional unit of 1 kWh of battery nominal cell capacity was chosen for the study as it captures the battery's main function, storing and delivering energy. Furthermore, it is a commonly used functional unit in LCA studies assessing batteries. Where environmental impacts of the materials alone are discussed, a functional unit of 1 kg material is used.

The main intended audience of this study is composed of researchers and manufacturers working with the development and production of battery materials and cells, and particularly those exploring the use of bio-waste derived resources. The study also aims to inform and provide inventory data and learnings to LCA practitioners working on bio-based materials, batteries, emerging technologies, and prospective analysis.

Future Scenario Development

For the future scenario development, we performed two types of analysis. First, we considered how the project KPIs and battery components in the foreground system individually affect the environmental impact of going from lab-scale (year 2025) to industrial-scale (year 2040). This allowed us to evaluate the effect of each parameter and served to make a priority list for developers. In the second analysis, we combined inventory parameters into cradle-to-gate scenarios to consider the combined effect. The analyses were performed using an explorative approach, with a worst-case and a best-case scenario for the parameters under study.

To establish inventory parameters, we took a two-step approach. First, we performed an analysis of political, economic, socio-cultural, technological, environmental, and legal factors (PESTEL analysis), following the framework from [29] to identify factors that may affect battery development in the cradle-to-gate perspective. Then, we drew a causal loop diagram to map out the most important interrelationships between key factors and essential inventory parameters. Figure 3 depicts the factors established in the PESTEL analysis, their interrelationships mapped out in the causal loop diagram, and the relation of key factors to inventory parameters. In the figure, solid lines denote positive relationships (e.g., higher resource prices increase battery costs), while dotted lines denote negative relationships (e.g., higher battery costs reduce market acceptance).

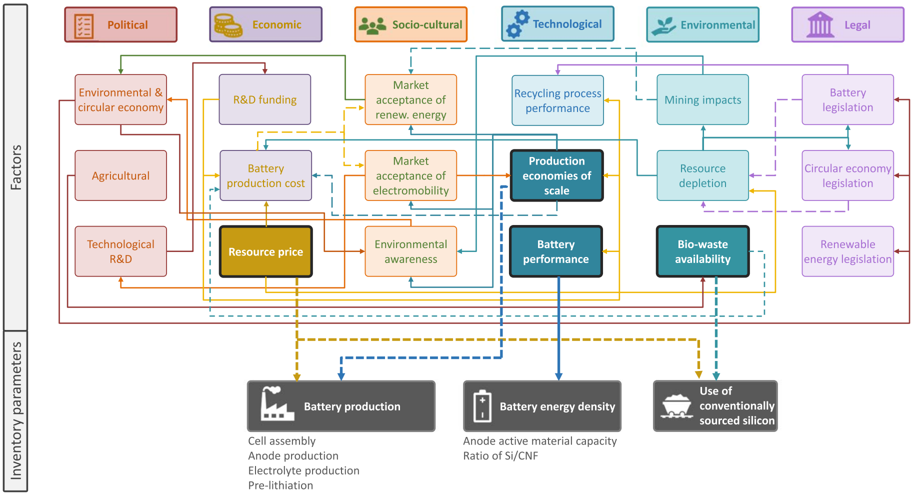

Fig. 3 PESTEL analysis identifying external factors and causal loop diagram connecting external factors and links between key factors and essential inventory parameters. Key factors are outlined and highlighted with a darker shade and have a link to essential inventory parameters

Based on the PESTEL analysis and causal loop diagram, we established four key factors that relate to different inventory parameters: resource price, production economies of scale, battery performance, and bio-waste availability. We identified resource price and production economies of scale as key factors related to battery production that are linked to four inventory parameters: cell assembly, anode production, electrolyte production, and pre-lithiation. These processes are all part of our foreground system, unlike the cathode which is part of the background system. Next, we found that battery performance in the cradle-to-gate perspective relates to energy density, which is directly influenced by two inventory parameters connected to the anode: anode active material capacity and the ratio of Si/CNF. Electrolyte conductivity, Li-ion transference number, and potential window also have a complex effect, but are not investigated here. All selected inventory parameters correspond to project KPIs. A combined analysis with two future scenarios was also constructed, representing worst- and best-case outcomes for the cells, within the parameters under study.

The PESTEL analysis additionally shows that resource price and bio-waste availability may lead to conventionally sourced Si replacing bio-Si. However, the source of Si is not an inventory parameter that may change as the battery technology matures but rather a supply chain aspect and was therefore not considered in the parametric analysis. In addition, no commercially porous Si is yet on the market, and conventional Si requires treatment to develop comparable morphology and functionality to bio-Si from barley husk.

The analysis structure is summarised in Figure S1 and Figure S2 in Supplementary Information A, and includes the following parameter and scenario variations:

- Lab-scale baseline: Derived from experimental data for 0.2 Ah pouch cells in year 2025.
- Industrial worst-case: A scaled-up baseline at 10 Ah pouch cell format in year 2040.
- Single-parameter optimised variations based on the industrial worst-case scenario, grouped by category

  Battery production processes:

    Cell assembly optimisation
    Electrolyte production optimisation
    Anode production optimisation
    Addition of pre-lithiation

  Anode energy density factors:

    Anode active material capacity optimisation
    Si/CNF ratio optimisation

- Industrial best-case: All investigated parameters optimised simultaneously for a 10 Ah pouch cell in year 2040.

Where the six single parameters were individually varied, they were varied between their industrial worst-case value to an assumed optimised industrial best-case value, allowing evaluation of individual effects for developers. In brief, the industrial worst-case was presumed to reflect a scaled-up version of the lab-scale process, with performance parameters expected at the end of the current project in 2025, whilst the ‘best-case’ represents a more optimised set of these parameters possible in year 2040. Pre-lithiation via a direct contact method was modelled as a parameter variation to explore its potential contribution to future large-scale LIB performance improvements [34]. It should be noted that the industrial best-case reflects a relatively optimistic but plausible scenario for the selected parameters under study, rather than an absolute best-possible level considering all battery cell parameters. Economic sustainability across scenarios, including changes associated with pre-lithiation, was not assessed within the study.

Life Cycle Inventory Modelling of Lab-Scale Production

This section details the foreground system modelling relating to production steps of the battery materials (bio-Si, anode, and electrolyte) shown in Fig. 4, as well as the battery cell at lab-scale. Process electricity use was estimated based on the equipment power rating, assumed average power output and energy efficiency, and operation duration. Complete inventory descriptions and data and summaries of production energy use estimates can be found in Supplementary Information A Section S1.2 and Supplementary Information B.

Bio-SiO_2 is produced from barley husk, a low-value bio-waste, and is used as a precursor for both bio-Si and electrolyte production. No agricultural burdens were allocated to the husk, consistent with a surplus allocation approach in which all burdens are assigned to the primary product (barley grain) [35]. Accordingly, only transport of husks from barley processing was included.

Barley husks were converted to bio-SiO_2 via acid leaching followed by calcination. Acid leaching was modelled using 10% hydrochloric acid, with spent acid treated as hazardous waste and no silicone oil consumption assumed due to reuse. A biomass yield of 50% was assumed, with the remaining biomass dissolved during leaching. The leached material was

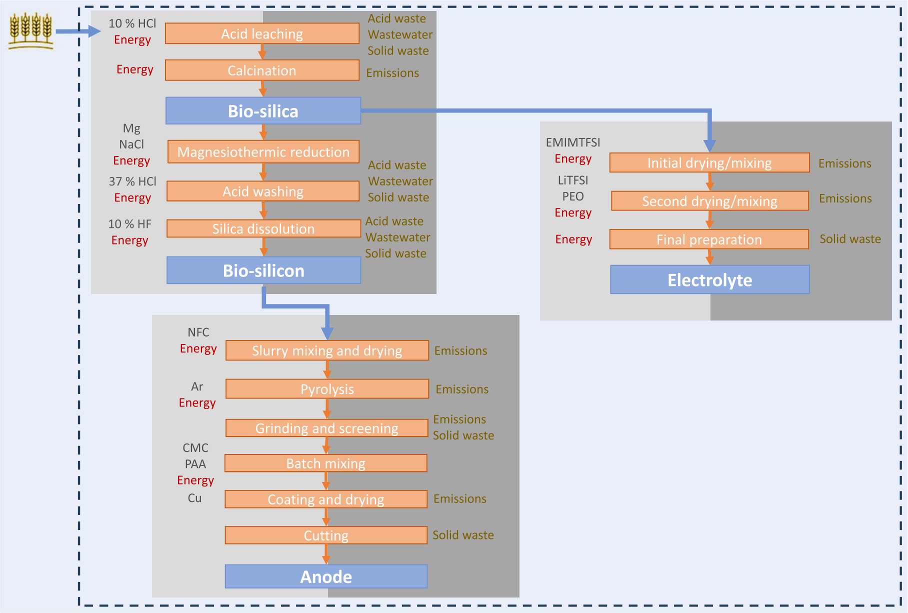

Fig. 4 Key steps at lab-scale to produce bio-Si, the Si/CNF anode, and the electrolyte used in the battery cell

dried and calcined at 600 °C, with biogenic CO_2 emissions from biomass burn-off treated as non-fossil. The conversion efficiency from barley husk to bio-SiO_2 was assumed to be 3%.

Bio-SiO_2 was converted to bio-Si through magnesiothermic reduction, acid washing, and dissolution of unreduced SiO_2. The process involved magnesium reduction under inert atmosphere, hydrochloric acid washing to remove magnesium, and hydrofluoric acid treatment to dissolve residual SiO_2, with all spent acids assumed to be collected and treated. The yield of bio-Si was approximately 20% relative to the reduced SiO_2 input, corresponding to an overall conversion efficiency of 0.6% from barley husk to bio-Si. Total electricity demand for bio-Si production was estimated at 37 kWh/g of bio-Si, reflecting high demands from lab-scale processing.

The anode was produced from bio-Si and CNF through slurry mixing, drying, pyrolysis, grinding, casting, and cutting. Anode compositions were parameterised and therefore modelled separately from process energy use. Pyrolysis under inert atmosphere constituted the dominant energy demand, and cutting losses of 20% were assumed. Production of a 320 g batch of Si/CNF slurry required approximately 2,800 kWh of electricity, driven by repeated high-temperature pyrolysis steps and small batch sizes.

Production of the bio-based electrolyte involved drying, mixing, solvent evaporation, and film formation using bio-SiO_2, polymer components, ionic liquid, and lithium salt, with proxy datasets applied where primary data were unavailable. Solvent recovery (80%) and material losses during film preparation (20%) and cutting (10%) were included. Total electricity demand for electrolyte production was estimated at 26 kWh/kWh of bio-SiO_2-based electrolyte.

Regarding assembly of materials into a cell, we sourced energy use data in cell manufacture from [36], normalised by cell capacity. Their analysis offers energy estimates for a range of Li-ion batteries as well as post Li-ion battery technologies, including solid-state batteries.

Life Cycle Inventory Modelling of Future Scenarios

The text below describes the inventory data for the industrial-scale foreground system modelling and focuses on individual parameter variations applied in the worst- and best-case analyses for battery production processes and anode energy density factors. Variations were thereafter combined to an overall best-case. As for lab-scale, detailed information and complete inventory data are provided in Supplementary Information A Section S1.2, and Supplementary Information B.

Battery Production Processes and Parameter Variations

Lab-scale battery production inventory models were scaled up to a worst-case industrial-scale, with further individual inventories developed for best-case optimised cell assembly, electrolyte production and anode production parameter variations. An additional pre-lithiation variant using stabilised lithium metal powder was included in the parameterised analysis to compensate for lithium losses during initial cycling, which are particularly pronounced for Si anodes, thereby improving initial capacity and cycle life.

Scale-up was primarily based on input from project technology developers. In the absence of industrial-scale data, literature values for current and future battery manufacturing energy use [36] and general scale-up guidance [37] were applied. Common scale-up assumptions were used across all processes, including material production volumes of 100 kg (worst-case) and 200 kg (best-case) and acid and solvent recovery where applicable. Additional reductions in energy use were assumed in selected cases within the best-case scenario, achieved through Pinch Analysis.

Future energy use for cell assembly, formation, and ageing was derived from [36] by applying worst- and best-case relative reductions to current energy use. Total future energy demand for cell manufacture was estimated at 0.9 and 0.4 kWh kWh^{-}1 cell capacity for worst- and best-case scenarios, respectively.

Battery Energy Density Inventory Parameters

Parameters relating to battery energy investigated in this work included two factors that relate to the anode: the anode capacity and the ratio of CNF to Si. When investigating the independent effect of these parameters at industrial-scale, we used the worst-case inventory models, but independently adjusted/optimised associated cell metrics (see Sect. "Cell metric data" for details). This meant that we assumed no changes in processes or material use, but that improvements stemmed from increased material properties leading to higher energy density. The worst-case scenario assumed that end-of-project KPIs relating to anode capacity and the ratio of CNF to Si were achieved without further improvement, while in the best-case these KPIs were exceeded. Regarding the anode capacity, we assumed that in a best-case scenario it can improve from 600 mAh/g to 900 mAh/g. For the ratio of CNF to

Si, affecting the trade-off between specific capacity and mechanical strength of the anode, we assumed this to decrease from 0.33:1 in a worst-case scenario to 0.25:1 in an optimised best-case scenario.

Cell Metric Data

Cell performance and composition were assessed for cells produced at lab and industrial scale under worst- and best-case scenarios, as well as for the six intermediate scenarios at industrial-scale with independently optimised parameters. A full break-down of cell performance and the composition in terms of different modelled components for the anode, electrolyte, cathode, pouch cell packaging, and stabilized lithium metal powder (if pre-lithiating) is given for all options in Section S1.3 in Supplementary Information A. Assumed anode and assembly scrap rates are also given for each option.

In summary, finished 0.2 Ah cells at lab-scale have a weight of 5.7 g (including 4% balance-of-cell weight, i.e., packaging, tapes, tabs, labels, etc.), a gravimetric energy density of 112 Wh/kg, and a cell energy capacity of 0.6 Wh. In the industrial-worst scenario, the finished 10 Ah cells are estimated to have a weight of 174 g (including 4% balance-of-cell weight), a gravimetric energy density of 116 Wh/kg, and a cell energy capacity of 20 Wh. In the industrial-best scenario with pre-lithiation and all parameters investigated relating to battery production processes and energy density factors improved, the cell weight is estimated to reduce to 142 g whilst the gravimetric energy density and cell energy capacity increase to 212 Wh/kg and 30 Wh, respectively.

Background System

Ecoinvent 3.10 was used as background system for extraction, production, and transport of materials, generation and transmission of electricity, production and distribution of heat, and generic waste treatment processes. Electricity supply was modelled using two generic scenarios for medium voltage: one based on natural gas (conventional power plant, Norway) and one on hydropower (grid connected reservoir in alpine region, Norway), representing ‘high-fossil’ and ‘low-fossil’ conditions respectively. We deliberately chose not to apply time-specific projections or integrated background changes, e.g., premise [30], as given the already high complexity of the study and its focus on parameters within the influence of technology developers, this would blur the distinction between technology-driven foreground changes and systemic background developments. Moreover, as we vary only a subset of potential technological improvements, we do not aim to precisely predict how the technology will perform in 2040 but rather illustrate the relative importance of selected parameters under contrasting electricity assumptions.

Where used, conventional Si LCIs were sourced from the *ecoinvent* database, reflecting established industrial-scale production. Conventional Si is produced via carbothermic reduction, where quartz (SiO_2) is reacted with coal or coke in electric arc furnaces to yield metallurgical-grade Si. This energy- and carbon-intensive process requires further refining to reach higher-purity grades such as solar-grade, from which battery-grade Si is typically derived. Given its heavy reliance on fossil inputs, the process is likely to undergo major changes in the future, including shifts to cleaner reductants, electrification, and/or alternative production methods. Accordingly, the conventional Si dataset cited here is not intended as a forward-looking technological baseline. Rather, it serves as a methodological upper-bound, offering a conservative benchmark for interpreting the relative performance of bio-Si and supporting early-stage learning about potential improvement trajectories.

Other details for background system processes can be found in Supplementary Information A, Section S1.4.

Life Cycle Impact Assessment

We considered four diverse midpoint impact categories to evaluate the environmental performance and hotspots of the materials. The four impact categories were: climate change, acidification, human toxicity (carcinogenic), and mineral resource depletion. Climate change impact in terms of global warming potential over a 100-year perspective, acidification, and human toxicity (carcinogenic) were estimated using the EF v.3.1 characterization method, while long-term mineral resource depletion was estimated using the crustal scarcity indicator [38]. All calculations were performed using the OpenLCA software version 2.3.1.

Results and Discussion

In this section analysis results are presented for both bio-Si and the full LIB cell, beginning with bio-Si due to its central role in the battery concept. Climate change impacts in terms of kg CO_2-eq are used to illustrate the contributions of individual production steps and to identify opportunities for improvement at industrial-scale. This is followed by the results for the full battery cell, where the broader set of environmental impact categories is assessed through the parametric and combined scenario analyses. To set the starting point for the industrial-scale scenarios, lab-scale production results are shown as a reference, reflecting un-optimised processes and small batch operation. Overall findings related to circularity and environmental sustainability are subsequently discussed.

Environmental Impacts of Bio-Silicon Production

Figure 5 compares the climate change impacts (kg CO_2-eq/kg Si) for the industrial-scale worst- and best-case scenarios of bio-Si, under varying electricity supply conditions with high (black bars) or low (grey bars) fossil content. For interest, an intermediate step is also shown between lab- and industrial-scale for a scenario whereby production has been scaled-up to industrial-worst levels, but acid, magnesium, sodium chloride, and solvent recovery have not been implemented.

Figure 5 shows that, as expected, lab-scale bio-Si exhibits the highest climate change impact, around 20,400 kg CO_2-eq/kg Si. In contrast, best-case industrial scenarios that incorporate selected improved processing and waste recovery efficiencies show substantial reductions, with the lowest impact around 50 kg CO_2-eq/kg Si with the use of low-fossil electricity . This use of low-fossil electricity is essential combined with the processing improvements to achieve highest climate change impact reductions. To provide a contextual anchor, conventional Si production datasets in *ecoinvent* report climate change impacts of 22 kg CO_2-eq/kg Si (Germany) and 31 kg CO_2-eq/kg Si (rest of world) for solar-grade purity, and 82 kg CO_2-eq/kg Si (Germany) and 116 kg CO_2-eq/kg Si (rest of world) for

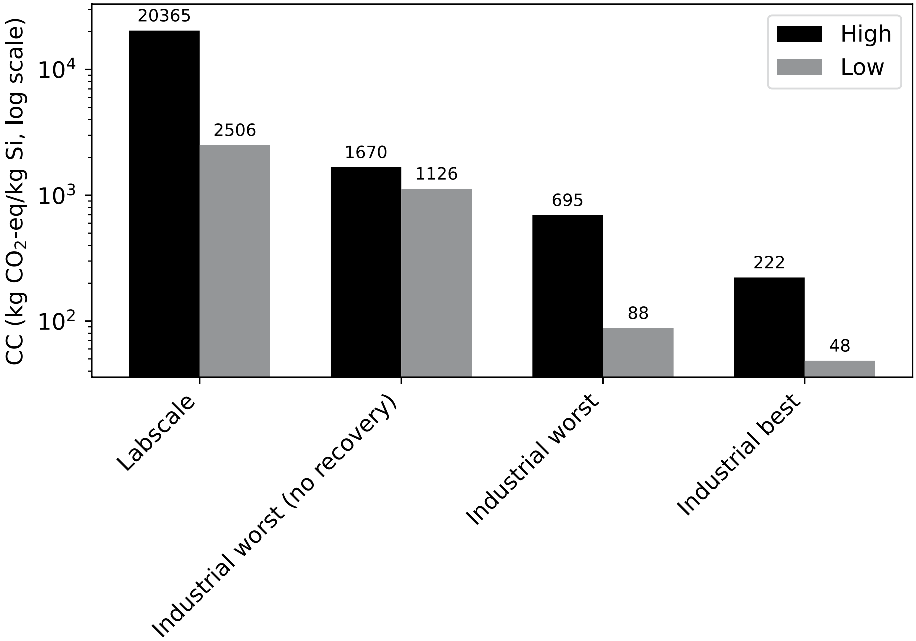

Fig. 5 Climate change (CC) impacts of bio-Si production (kg CO_2-eq/kg Si) at lab-scale production and at industrial worst- (with and without recovery of acids and materials) and best-case, plotted on a log-scale. High and low reflect electricity with high or low fossil content, respectively

electronics-grade purity. These are not intended as a direct comparative benchmark for substitution, but to help position the bio-Si results within the broader landscape of existing Si technologies. For reference, the bio-Si produced is expected by material developers to have a quality level between solar- and electronics-grade conventional Si, although the porosity of the bio-Si means it is not directly comparable in terms of functionality. To use commercial Si in the battery would require e.g. electrochemical etching with hydrofluoric acid to generate the needed porosity, adding to climate change impacts.

Figure 6 presents a contribution analysis of climate change impacts (kg CO_2-eq/kg Si) by process across the four bio-Si production scenarios (lab-scale, scaled-up without recovery, industrial-worst, and industrial-best) based on the low-fossil electricity mix. This electricity scenario was selected to isolate and better reflect the relative influence of process steps and material flows on total climate change impact.

Figure 6 highlights how environmental hotspots shift along the technology maturity trajectory from lab to industrial-scale using the low-fossil electricity mix. At lab-scale, the main contributors to climate change impacts are acid waste (33%), wastewater (19%), tap water (15%), and electricity (12%), reflecting the waste- and energy-intensive nature of early-stage processing. As the process is scaled up without waste recovery, acid waste becomes the dominant hotspot (61%), underscoring the importance of optimizing acid use, recovery, and treatment strategies. With acid recovery implemented at industrial-scale, the main contributions shift to resource inputs such as magnesium, although acid waste is still a significant contributor. A contribution analysis by production step was also performed (Figure S3 in Supplementary Information A), showing the shift from acid-waste intensive processes

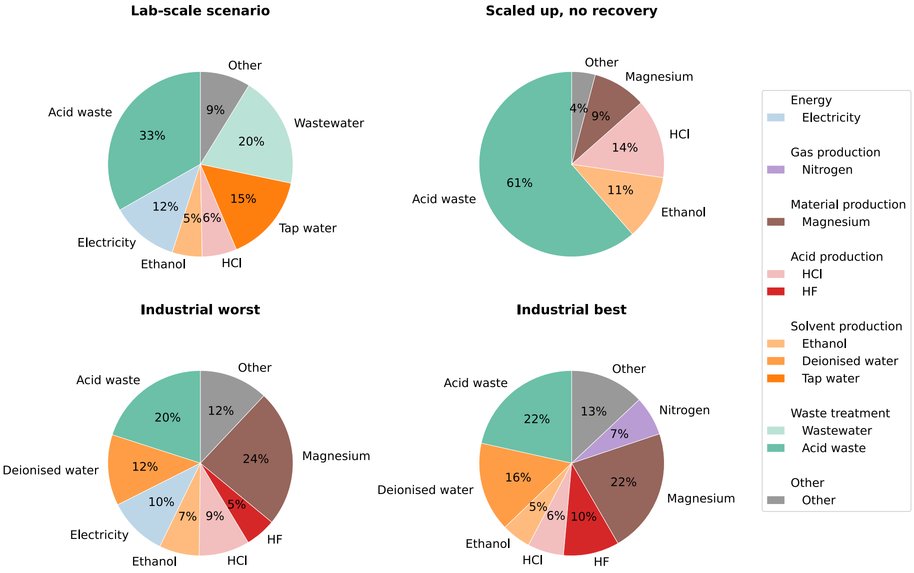

Fig. 6 Climate change contribution analysis of bio-Si production (% contribution to total kg CO_2-eq) by process type across four scenarios: lab-scale, scaled-up without recovery, industrial-worst, and industrial-best. Results are shown for the low-fossil electricity mix. Contributions below 4% are grouped as ‘other’. Hydrofluoric acid is denoted HF on the figure, and hydrochloric acid is denoted HCl

(e.g., SiO_2 dissolution and acid washing) to resource-intensive processes (e.g., magnesiothermic reduction) as key climate change impact contributor from lab to industrial-scale.

Although electricity plays a smaller proportional role at industrial-scale when using low-fossil electricity, total energy demand per unit of bio-Si remains substantial. At lab-scale, the process requires around 37,000 kWh/kg bio-Si produced, reflecting low yields and inefficient batch processing. When scaled up to worst-case at industrial-scale (both with and without material or acid recovery), electricity demand drops to around 1,100 kWh/kg Si, and further to around 240 kWh/kg Si under the best-case industrial scenario. High electricity needs explain the necessity for renewable energy seen in Fig. 5, demonstrating continued need for electricity use optimisation, energy efficiency measures, and process development.

Improving yields is a key route to reducing processing requirements. Current conversion efficiencies are low, ranging from 0.6% at lab-scale and in the industrial best-case, to 0.4% in the industrial worst-case. In the latter, the calcination yield was assumed to drop from 6 to 4% to account for potential inefficiencies in heat transfer and reaction uniformity at larger scales, while yields in other processing steps were kept constant. Losses occur at several stages: at lab-scale, 50% of the biomass mass is lost during acid leaching, only 6% of the remainder is converted to bio-SiO_2 via calcination, and just 20% of that is reduced to bio-Si. As a result, producing 1 kg of bio-Si requires 167 kg of barley husk at lab-scale and in the industrial best-case, and 250 kg in the industrial worst-case. One option to improve yields is selecting feedstocks with higher SiO_2 content, such as rice husk, which contains up to 20% SiO_2 [39].

Environmental Impacts of Battery Pouch Cell

Regarding cell impacts, climate change results per 1 kWh battery pouch cell are presented for combined parameter scenarios at industrial worst- and best-case scales, with the lab-scale result included as a starting-point reference for scale-up (Fig. 7).

Under a low-fossil electricity mix, the best-case industrial scenario results in around 60 CO_2 kg-eq/kWh using the bio-Si, increasing to around 190 kg CO_2-eq/kWh under a high-fossil electricity mix. For context, median cradle-to-gate LIB cell footprints in the literature typically fall around ~ 50–120 kg CO_2-eq/kWh [40], with 78 kg CO_2-eq/kWh cell for LFP-based cells specifically [41]. These results are only used here only as today's benchmark. Conventional Si is not employed alternatively in the cell as a reference here due to a lack of direct functionality comparability with the porous bio-Si.

The analysis shows that electricity source has a pronounced influence on climate change impacts; at industrial best-case scale, shifting from low- to high-fossil electricity mix increases impacts by approximately a factor of 3, while at lab-scale, emissions rise by a factor of around 13. This reinforces the importance of aligning process development with energy system decarbonisation. Due to these results, bio-Si is combined with low-fossil energy for subsequent analysis in this section, also ensuring that differences primarily reflect material and process design choices. In addition, the no-recovery scenario, which is not realistic at industrial-scale, is not included.

Results for the battery pouch cell for three added impact categories in addition to climate change (acidification, human toxicity (carcinogenic), and long-term mineral resource

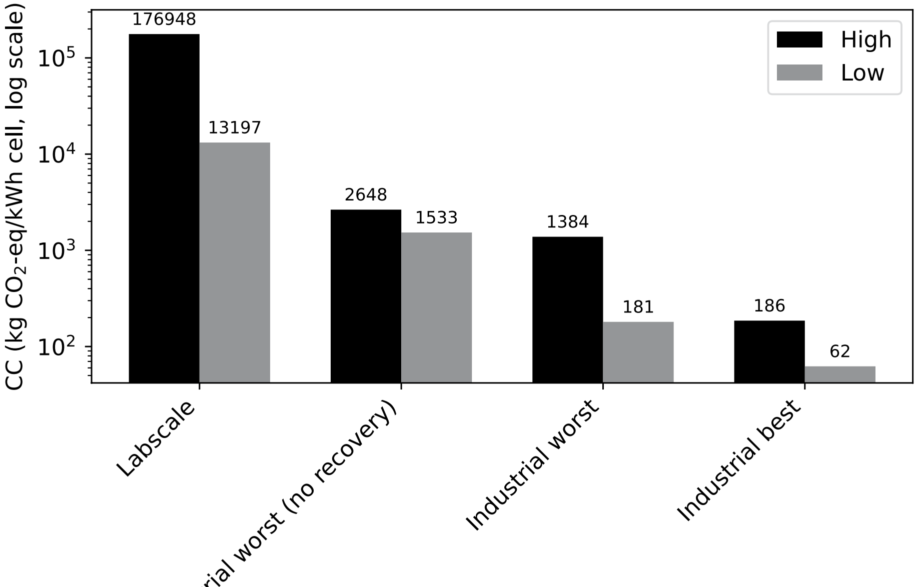

Fig. 7 Climate change (CC) impacts of battery pouch cell production (kg CO_2-eq/kWh cell) at lab-scale production and at industrial worst- (with and without recovery of acids and materials) and best-case, plotted on a log-scale. High and low reflect electricity with high or low fossil content, respectively

depletion) are presented in Fig. 8 per kWh cell, normalized to the highest value. Lab-scale results were excluded for visual clarity. Each bar represents the cumulative effect of individual improvement measures, grouped into the two categories: (1) production improvements (electrolyte production, anode production, cell assembly, and pre-lithiation), and (2) battery energy density improvements (anode active material capacity increase and Si/CNF ratio optimization). The black bars correspond to the industrial worst-case (normalized to 100%), while the green bars represent the full industrial best-case, where all parameters are optimized simultaneously. The intermediate bars in blue and grey indicate the effect of improving only one parameter (to production or anode energy density, respectively), while all other parameters remain at worst-case settings.

Figure 8 shows that the influence of each parameter varies across impact categories. Among the parameters tested, increasing anode capacity is the most influential overall, reducing burdens across all categories. Higher specific capacity increases the energy stored per unit mass, which directly lowers material and energy requirements per kWh of cell energy. Improvements in anode production (through equipment optimisation, acid and material recovery, and other process refinements) have the greatest effect on human toxicity (carcinogenic), largely because magnesium production, a key input to bio-Si synthesis, dominates this category (49% contribution for the industrial-worst scenario). Reducing magnesium demand through production optimisation is therefore particularly important. Optimising cell assembly and manufacturing most strongly affects long-term mineral resource depletion, as copper current collectors are the largest contributor (39% contribution for the industrial-worst scenario). In the best-case manufacturing scenario, the anode is assumed to be self-supporting and requires no copper, significantly reducing this burden. Pre-lithiation is also influential, both because it compensates for initial lithium losses and because it increases gravimetric energy density; its environmental promise has also been

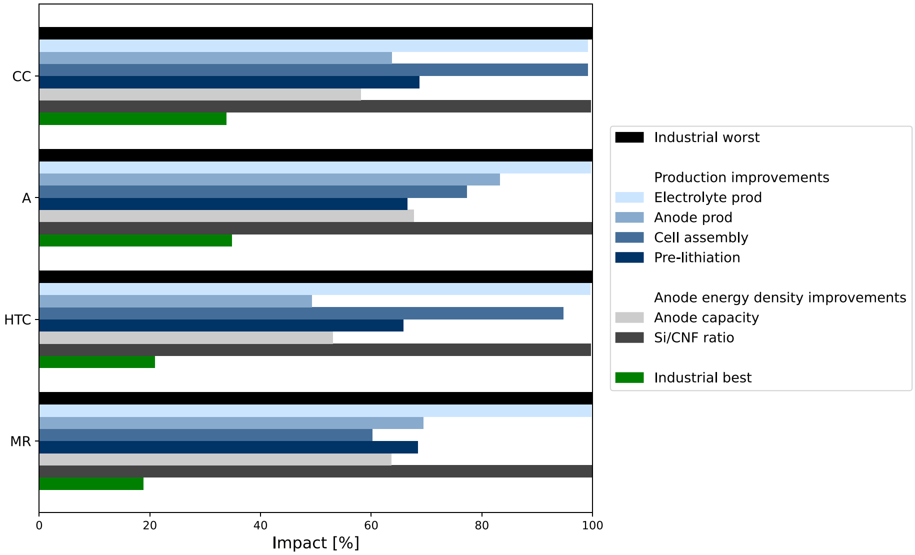

Fig. 8 Normalised climate change (CC), acidification (A), human toxicity carcinogenic (HTC) and long-term mineral resource depletion (MR) at industrial-scale for the parametric and combined scenario analyses for the full battery cell, per kWh. Results are shown for the low-fossil electricity mix

highlighted by [42]. In contrast, optimisation of electrolyte production and adjustments to the Si:CNF ratio (already low) had negligible effects. Overall, while multiple improvements are needed to achieve the industrial best-case, targeted changes in anode design emerge as particularly critical for reducing environmental impacts.

Since several of the evaluated parameters directly affect the cell's energy capacity, and thus the normalization of impacts per kWh, we also normalized per kg and per cell as an extension (Figure S4). For anode capacity, reductions in impact appear smaller when expressed per kg or per cell than per kWh. If not normalised by cell functional energy delivery, then due to the addition of stabilized lithium metal powder, pre-lithiation increases impacts per kg and per cell. These findings underscore the importance of selecting a functional unit aligned with the intended performance outcomes when evaluating emerging battery technologies.

To explore contributions in greater detail, Fig. 9 presents the component-level breakdown of environmental impacts per kWh across the parametric and combined scenario analyses.

The analysis shows that anode production is a major contributor to all impact categories, but particularly for human toxicity (carcinogenic) and long-term mineral resource depletion. The cathode contributes most significantly to acidification impacts, particularly (sharewise) for the industrial best-case with improvements to the anode, due to emissions of ammonia to air from the use of di-ammonium phosphate during LFP production. Contributions from the electrolyte and other components (pouch and assembly processes) are minimal. This figure ties in with parameterised findings and again shows that most of the environmental improvement potential lies within the anode design and related functional performance, while other cell components offer more limited scope for impact reduction under the conditions assessed.

Breaking down the anode contribution to climate change impacts by component revealed distinct differences between the bio-Si and anode processing. In the industrial best-case, bio-Si contribution was 89% and anode processing (excluding resource additions) 1%, whilst at the lab-scale, bio-Si contribution was 60% and anode processing 40%. Further investigation determined that the argon and energy needs for pyrolysis were key contributors at lab-scale, which reduced at industrial-scale due to optimisation of processing capacity (Figure S5).

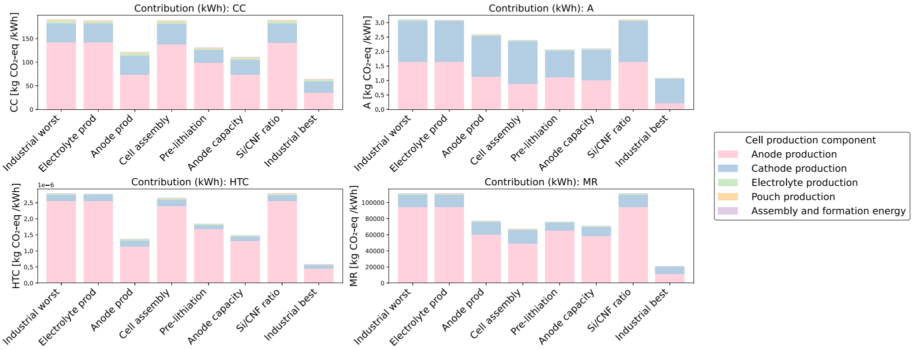

Fig. 9 Component-level contributions to environmental impacts per kWh for four selected impact categories: climate change (CC), acidification (A), human toxicity (carcinogenic) (HTC), and long-term mineral resource depletion (MR) at industrial-scale for the parametric and combined scenario analyses for the full battery cell. Results are shown for the low-fossil electricity mix

Accounting for all anode production steps, Fig. 10 shows the breakdown of anode climate change impacts by process type for the full anode production, including all components. At lab-scale, impacts are dominated by gas production (argon), waste treatment processes and electricity input, reflecting the high inert atmosphere and waste-intensive nature, as well as high energy requirements of early-stage synthesis. In the industrial cases, key contributors are material production (from inputs such as magnesium and sodium chloride) and waste treatment. The higher energy contributions at industrial-scale derives mostly from bio-SiO_2 calcination and are discussed in detail in Sect. "Sustainability and circular-economy implications".

Processing Factors Most Affecting Environmental Impacts

To assess the sensitivity of environmental impacts to uncertainty in key production assumptions, four parameters were selected for individual variation: acid input/output ratio, assembly scrap rate, anode scrap rate, and combined electricity input to material production and cell assembly. These parameters represent key contributors to system-level emissions in prior scenario and contribution analyses but also represent areas of high uncertainty in early-stage system modelling. Each parameter was individually varied from 0.5 to 1.5 times its baseline value, using the best-case industrial scenario with bio-Si as the reference, and both a high-fossil and low-fossil electricity input.

Figure 11 shows the resulting variation in climate change impacts. Under a high-fossil electricity mix (b), electricity input is the dominant contributor to variation, with a range approaching ± 70 kg CO_2-eq/kWh, reflecting its role as a primary contributor. Under the low-fossil electricity mix (a), the anode scrap rate and quantity of acid input/output becomes the key contributors to variation (± 20 kg CO_2-eq/kWh).

Sustainability and Circular-Economy Implications

The results of this study illustrate that environmental sustainability and circularity in emerging bio-based LIB technologies are not necessarily aligned. While the use of biogenic and waste-derived feedstocks can reduce reliance on virgin resources and align with circular

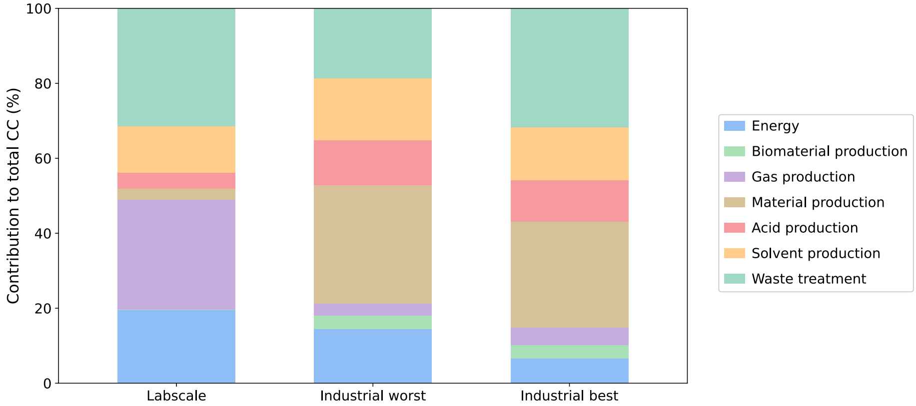

Fig. 10 Contribution analysis breakdown by process type of anode climate change (CC) impacts (% contribution to total kg CO_2-eq) across three anode production scenarios: lab-scale, industrial worst-case, and industrial best-case. Results are shown for the low-fossil electricity mix

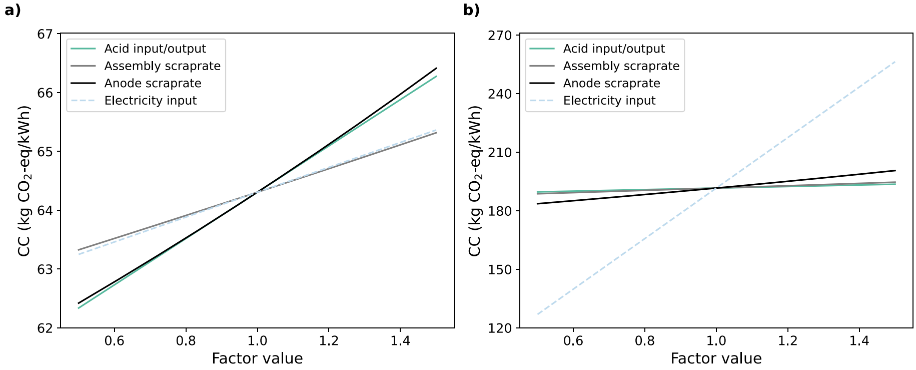

Fig. 11 Sensitivity analysis of climate change impacts for the industrial best-case battery cell using bio-Si, under (**a**) low-fossil and (**b**) high-fossil electricity mixes. Four key parameters were independently varied by ± 50% of their baseline values (scaling factor 0.5 to 1.5): acid input/output ratio, anode scrap rate, assembly scrap rate, and electricity input in production and assembly. The analysis shows the resulting variation in total climate change impacts (kg CO_2-eq/kWh). Note that the y-axes are not aligned

economy objectives, system environmental impacts are determined by energy demand, material efficiency, chemical intensity, and the effectiveness of recovery and reuse pathways across the full life cycle. Although potential reductions in environmental impact exist, as reported in previous LCA studies for bio-carbon production for energy storage devices [14] and bio-SiO_2 production [13], these are dependent on processing, region and feedstock characteristics [13].

Energy and material use emerge as key contributors to environmental impacts, particularly for lab-scale and early industrial-scale configurations. This relates to high electricity requirements associated with thermal processing steps, with climate and resource impacts amplified when supplied by carbon-intensive energy mixes. The reliance on hydrochloric and hydrofluoric acids introduces substantial material flows and hazardous waste streams, making system environmental sustainability also dependent on efficient recovery and reuse. While closed-loop recovery of acids, solvents, and salts can substantially reduce net environmental burdens, these recovery processes themselves require additional energy and infrastructure.

Although not evaluated in this study, overall system circularity can be reduced by additional resource inputs even when bio-waste feedstocks are used. For example, the Material Circularity Indicator (MCI) evaluates the share of recycled or biodegradable material inputs, recycling efficiency, and unrecoverable waste [43–45], meaning that high auxiliary material use or low recovery efficiencies can offset the circular benefits of waste-derived feedstocks. A review [43] further shows that some circularity indicators explicitly incorporate energy-related metrics, including energy use and the share of renewable energy, as demonstrated for example in [46].

Energy is a key resource, making its use an important metric in its own right; it was therefore analysed in further detail for cell production in this study. Figure 12 shows a Sankey diagram where energy inputs were disaggregated across different components (anode, electrolyte, cathode, and assembly) across combined cell production scenarios at lab- and industrial-scale. Flow widths are proportional both within and across figures. Anode energy contributions are further disaggregated by process type.

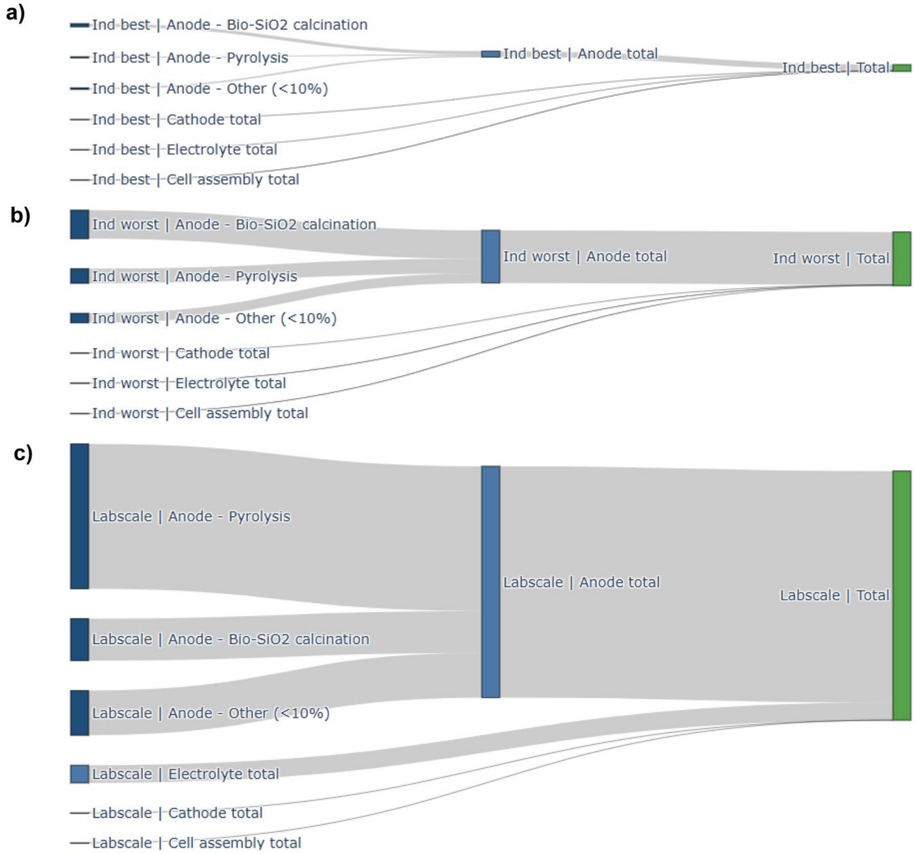

Fig. 12 Sankey diagram showing energy inputs from different production processes to produce 1 cell at **a**) industrial best-case (Ind best), **b**) industrial worst-case (Ind worst), and **c**) lab-scale. Flow widths are proportional to each other. Anode production processes contributing less than 10% of the anode total have been summed for clarity

Figure 12 shows thermal processing steps associated with anode production to be a dominant energy contributor at all scales. At lab-scale, pyrolysis is most intensive due to its 900 °C requirement and long processing times, while at industrial-scale the main burden shifts to calcination, as pyrolysis is assumed to operate continuously with shorter residence times and no ramp-up. Even with improved integration, Si/NFC pyrolysis, SiO_2 calcination, and SiO_2 dissolution (driven by distillation for waste recovery) remain major energy demands. Overall values are sensitive to assumptions on equipment power and operating times at industrial-scale, which carry considerable uncertainty.

Total energy use for battery cell production is large, even at simulated industrial-scale. Per kWh battery cell, the energy input for all material production and cell assembly was around 207 kWh in the industrial best-case, 2,470 kWh in the industrial worst-case, and 400,000 kWh at lab-scale. For comparison, energy use at a giga-factory producing conventional LIBs has been estimated at around 100 kWh/kWh cell, with further reductions expected as efficiency measures are implemented.

Energy (and material) demand also interact closely with other circularity dimensions. Current conversion efficiencies from barley husk to bio-Si are low, requiring large quantities of biomass per unit of active material. With low yields, upstream logistics, processing, and auxiliary energy and material requirements are effectively cumulatively increased per functional unit, reducing environmental benefits of utilising waste biomass inputs. These findings highlight that optimising process energy and material needs together with access to low-carbon electricity are necessary, but that process conversion efficiency is also a bottleneck for achieving environmentally sustainable circular systems.

Conversion efficiency is not only linked to system design but also to feedstock choice. Barley husk offers advantages in terms of availability and low upstream environmental burden, but its relatively low silica content limits achievable material yields. Alternative residues with higher SiO_2 content, such as rice husk (as used by [13, 39]), may improve material efficiency and reduce energy demand per unit of product. This highlights the need to assess waste and bio-waste streams not only on availability, but also on functional suitability and system-wide implications.

Consideration of co-production systems can also increase environmental sustainability, with for example, management and utilisation of bio-energy released during biomass feedstock combustion showing environmental benefits in [13]. Pyrolysis also releases biogenic CO_2, which although treated as carbon neutral in this model, could provide opportunities to lock down carbon flows.

Overall, the analysis demonstrates that bio-based pathways can shift environmental burdens from resource extraction to energy use, chemical processing, and recovery systems if not carefully designed, potentially reducing overall environmental sustainability. pLCA provides a critical framework for identifying these trade-offs early, enabling technology development pathways that simultaneously reduce environmental impacts and embed circularity through improved yields, lower chemical intensity, and integrated recovery systems. These findings point to the need for targeted efficiency improvements in high-temperature anode processing, either through optimisation or consideration of alternative materials or processing routes, with recovery and utilisation of bio-energy where possible. In addition, quantification of system circularity should be carried out using circularity indicators, in parallel to the LCA work.

Learnings for Further Prospective LCA on Emerging Material Technologies

This study highlights several uncertainties as well as methodological and practical considerations that are relevant for future pLCA applications, particularly those focused on emerging material technologies.

Firstly, although established frameworks exist for scaling up lab-scale data to industrial-scale processes, their practical application can be challenging. Uncertainties created by data gaps, inconsistent process descriptions, and variability in laboratory practice complicate the translation of lab-scale parameters into credible industrial-scale models. In this work, certain assumptions, such as reaction yields, batch-to-continuous transitions, and integration of recovery loops, required careful judgement and iterative validation, showing needs for transparent reporting and critical reflection in similar studies. High uncertainty has also been previously related to assumptions and process scale-up based on lab-scale data [18, 19].

Secondly, the lack of standardized guidance on equipment sizing and power requirements for different process types represents a major limitation. Although energy is found in this study to be a key contributor to environmental impacts, current estimates rely on power ratings rather than direct measurement, highlighting needs for more robust empirical data on equipment energy use or further generic, empirically derived rules of thumb for extrapolation of equipment energy use across TRLs. Access to benchmark data from primary industry sources, particularly for energy-intensive unit operations such as pyrolysis and calcination, would greatly enhance the reliability of energy input modelling at scale. In the absence of such data, uncertainty ranges remain wide. This work also highlights the value of involving chemical engineers alongside material scientists in low-TRL projects, even at early stages, to strengthen process realism for this type of assessment.

As indicated widely elsewhere, comparisons with conventional technologies should be approached with caution, as current industrial processes may not reflect the kinds of mature technologies that will be available in the future [18, 19]. However, we consider such technologies useful as upper-bound benchmarks, offering a reference point for the likely worst-case environmental impact under mature, scaled-up conditions. When included only for this purpose, as in the case of conventional Si or energy use for cell production in this study, this framing should be made explicit to avoid over-interpreting their relevance for future best-available alternatives.

Conclusions

This prospective cradle-to-gate LCA of a novel bio-Si-based lithium-ion battery cell demonstrates both the opportunities and challenges associated with using bio-waste as a feedstock for next-generation LIB materials. While barley husk bio-waste enables production of functional porous silicon with minimal upstream burdens, current processing routes are energy- and chemically intensive. With low-fossil electricity, lab-scale GHG emissions of 13,200 kg CO_2-eq/kWh cell decrease to 181 kg CO_2-eq/kWh in a modelled industrial worst-case and to 62 kg CO_2-eq/kWh in an optimised scenario. This best-case represents an optimistic yet plausible outcome for the selected parameters rather than an absolute upper bound across all aspects of battery performance. Nevertheless, even in this scenario, energy demand (207 kWh/kWh cell) remains roughly double that of conventional giga-factory production, highlighting the need for substantial process innovation.

From a circularity and sustainability perspective, the results show that circular feedstocks do not inherently deliver environmentally sustainable outcomes. Although bio-waste reduces reliance on virgin resources and aligns with circular-economy objectives, low material yields, high chemical intensity, and energy-intensive processing can shift burdens from extraction to processing and recovery systems. In this case, conversion efficiencies from barley husk to bio-Si remain below 1%, requiring large biomass inputs per unit of active material and limiting net circular benefits. Environmentally sustainable and circular performance are therefore closely linked to yield improvements, reduced chemical throughput, and effective recovery of acids and auxiliary materials. Feedstock choice also plays a critical role, as residues with higher SiO_2 content could substantially improve material efficiency and reduce cumulative energy demand.

With relevance to technology developers, the findings indicate that environmental viability depends primarily on improvements in process efficiency, yield, and resource recovery rather than feedstock substitution alone. High-temperature anode processing steps, notably Si/NFC pyrolysis and SiO_2 calcination, dominate energy demand, raising concerns from an energy resource perspective and showing needs for more efficient equipment, higher-yield routes, and access to renewable electricity. Acid recovery and reuse are also key : without recovery, acid waste (particularly hydrochloric acid) becomes a dominant hotspot. Recovery or substitution of magnesium and sodium chloride is similarly essential, with alternatives needed where recovery is not feasible. Acid and material recovery must be integrated directly into the anode processing chain rather than treated as downstream or add-on mitigation options. Within the anode, increasing active-material specific capacity, applying pre-lithiation, and optimising production processes deliver the largest improvements by simultaneously enhancing functional performance and reducing energy and material intensity. Finally, alternative bio-waste feedstocks with higher SiO_2 conversion rates, or routes that could generate useful co-products, could further reduce burdens. Once other parameters are optimised, strategies for hydrofluoric acid recovery may represent an important next step.

For LCA practitioners, the study highlights ongoing methodological challenges in prospective assessment of low-TRL technologies, including scaling laboratory data to industrial conditions under high uncertainty, limited process transparency, and the lack of standardised guidance for equipment sizing and energy use in energy-intensive unit operations. Given the sensitivity of results to energy and yield assumptions, transparent reporting, explicit scenario framing, and access to empirical benchmarks across TRLs are essential. Greater integration of chemical-engineering expertise alongside materials research can strengthen both process realism and the robustness of early-stage environmental assessments.

Taken together, the findings support a targeted sustainability-oriented development strategy focused on improving efficiency, optimising yields, and integrating recovery systems from the outset. Bio-waste has potential as a feedstock for novel LIB materials with increased circularity, but realising this potential depends on advances in process design and data quality rather than material sourcing alone. Circularity, and its contribution to environmental sustainability, must be evaluated at the system level, explicitly accounting for energy use, material efficiency, and recovery pathways across the life cycle.

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Data availability The authors confirm that the input data for the study are available within the supplementary materials. Further information can be available upon request.

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