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Online Supplementary Information

Life cycle assessment of sodium-ion batteries

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In this supplementary document, the complete LCI data is disclosed explicitly for reproducibility purposes. Furthermore, the LCA results and those of the sensitivity analysis are provided in tabulated form.

Battery layout

The battery layout is derived from technical datasheets for a commercial prototype layered oxide Na-Ion battery cell in an 18650 cell case [1]**.** There, the dimensions of separator, anode and cathode and their coating thicknesses (active material) are provided, what allows for calculating the battery composition on a mass basis. The amount of electrolyte is then calculated based on the internal volume of an 18650 cell and the volumes of anode, cathode and separator, giving 4,600 mm^3 of electrolyte. For the battery cell casing, technical data from a commercial provider of nickel plated steel battery cases is used [2]. Densities for electrolyte and separator are obtained from literature [3–5]. The obtained battery mass composition is provided in Table S1. The battery cell has an estimated energy density of 128 Wh·kg^{-1}, using a layered oxide cathode material and a hard carbon based anode [1]. As binder for the anode material, styrene- butadiene rubber (SBR) in combination with carboxymethyl cellulose (CMC) is used [6,7], while the cathode is prepared with polyvinylidenfluoride (PVdF) as binder.

Table S1. Composition of an 18650 type SIB cell

Part	Function	Material	Amount		Share
Anode	Active material	Hard carbon	8325.75	mg	20.6%
	Conductive carbon	Carbon black	269.30	mg	0.7%
	Binder	SBR/CMC	359.06	mg	0.9%
	Collector foil	Aluminium	1434.51	mg	3.6%
Cathode	Active material	Layered oxide	11970.38	mg	29.6%
	Conductive carbon	Carbon black	254.69	mg	0.6%
	Binder	Polyvinylidenfluoride	509.38	mg	1.3%
	Collector foil	Aluminium	1276.13	mg	3.2%
Separator	Separator	Polyethylene foil	815.10	mg	2.0%
Electrolyte	Electrolyte	Sodium hexafluorophosphate based	5643.00	mg	14.0%
Housing	18650 container	Nickel plated A3 steel	9300.00	mg	23.0%
	Sealing	Nylon	200.00	mg	0.5%
Sum	**18650 battery cell**		**40379.74**	**mg**	100.0%

Life cycle Inventories (LCI)

Na-Ion battery pack

The battery pack is assumed to be of a similar layout like that of Li-Ion batteries (LIB). The life cycle inventory (LCI) for the battery pack is thus derived from existing life cycle assessment (LCA) studies on Li-Ion batteries, where the battery cells make up around 80% of the weight of the whole battery pack, the casing 14.5% (steelbox type) and the battery management system (BMS) 5.5% [8–10]. Table S2 shows the corresponding LCI. The energy density of the battery pack is 102 Wh·kg^{-1}. Since no established large scale industry for sodium-ion battery (SIB) production yet exists, it is assumed that production takes place majorly in Europe and transport distances are estimated accordingly, based on the standard transport distances according to the ecoinvent standards [11]. The BMS is assumed to be manufactured together with the battery pack and requires no further transport.

Table S2. LCI for an SIB battery pack

Item	Dataset	Amount	Unit
Inputs			
Battery cell	Battery cell, Na-Ion, NMMT-HC, 18650, at plant	7.99E-01	kg
Steelbox, material	Market for reinforcing steel	1.45E-01	kg
Steelbox, production	Market for sheet rolling, steel	1.45E-01	kg
BMS	Battery management system	5.60E-02	kg
Electricity	Medium voltage, market group - EU	3.53	kWh
Infrastructure	Metal working factory construction	4.58E-10	unit
Transport, lorry	Lorry, >16t, Euro 5, RER	1.00E-01	t·km
Transport, train	Market for freight train, EU	5.42E-01	t·km
Outputs			
Waste heat	Heat, waste, to air	12.72	MJ
Battery pack	Na-Ion battery pack, NMMT-HC, 18650, at plant	1.00	kg

Battery management system (BMS)

The LCI for the BMS is directly taken from Notter et al. [8], which was found to provide the most sound inventory data for battery management systems among existing studies disclosing the LCI for the BMS. In fact, the modelling of the BMS is a critical aspect for the LCAs, since electronic parts show high relative impacts in several categories and thus the associated impacts vary strongly depending on how the BMS is modelled. The BMS as modelled by Notter is the one with the lowest impacts when comparing existing LCA studies [3,5,8–10,12] and thus the one that least affects the final results. Table S3 provides the LCI for the BMS.

Table S3. LCI for a battery management system (BMS)

Item	Dataset	Amount	Unit
Inputs			
Electronics	Market for printed wiring board, surface mounted, unspecified, Pb containing	1.81E-02	kg
Electronics	Market for printed wiring board, surface mounted, unspecified, Pb free	4.23E-02	kg
Data cable	Market for cable, data cable in infrastructure	6.66E+00	m
3 phase cable	Market for cable, three-conductor cable	4.46E-01	m
Transport, lorry	Lorry, >16t, Euro 5, RER	0.093957	t·km
Transport, train	Market for freight train, EU	0.56374	t·km
Outputs			
BMS	Battery management system	1.00	kg

Na-Ion battery cell

The LCI for the SIB cell is given in Table S4. Heat and electricity demand during battery manufacturing are critical aspects that significantly influence the final results, while varying strongly among different studies [13]. It is assumed that (on a per kg basis) the manufacturing of SIBs uses the same processes like LIBs and thus the electricity and heat demand during cell and battery pack manufacturing are identical. In order to increase comparability with existing LCA studies on LIBs, the LCI of the principal studies are recompiled and the same energy demand for cell and battery pack manufacturing is assumed. The mean value obtained from all studies that use own original LCI and disclose these in a sufficiently transparent way is taken [3,5,8–10,12]: 6.44 kWh of electricity and 21.02 MJ of heat per kg of battery pack. The distribution of the electricity demand between cell and pack manufacturing process is assumed to be identical to that used by Notter et al. [8], while heat is required only for the cell manufacturing process. For estimating transport distances, standard distances for chemical products are used according to the ecoinvent guidelines [11], assuming that cathode, anode and electrolyte are produced on site and thus do not require transport. A 5% loss (discarded cells due to insufficient quality) is accounted for according to the ecoinvent guidelines and in concordance with the work of Notter et al. [8,11].

Table S4. LCI for 1 kg of Na-Ion battery cell

Item	Dataset	Amount	Unit
Inputs			
Cathode	Cathode, NMMT layered oxide, for Na-Ion battery	2.70E-01	kg
Anode	Anode, hard carbon-Al, for Na-Ion battery	3.65E-01	kg
Separator	Market for battery separator	2.12E-02	kg
Electrolyte	Electrolyte, $NaClO_4$ based, for Na-Ion battery	1.47E-01	kg
Cell container	Cell container, 18650 type, for battery	2.47E-01	kg
Nitrogen	Market for nitrogen, liquid	1.05E-02	kg
Infrastructure	Market for chemical factory, organics	4.00E-10	p
Electricity	Medium voltage, market group - EU	3.64	kWh
Heat	Central or small scale, natural gas - EU	26.31	MJ
Transport, lorry	Lorry, >16t, Euro 5, RER	4.20E-02	t·km
Transport, train	Market for freight train, EU	2.50E-01	t·km
Outputs			
Waste heat	Heat, waste, to air	4.69E-01	MJ
Waste parts	Market for used Li-ion battery	5.00E-02	kg
Battery cell	Battery cell, Na-Ion, NMMT-HC, 18650, at plant	1.00	kg

Cell container

The LCI for the 18650 cell container is based on a technical datasheet from a provider of empty 18650 cell cases [2]. Transport distances are estimated according to the ecoinvent guidelines [11]. Table S5 provides the corresponding LCI.

Table S5. LCI for 1 kg of 18650 cell container

Item	Dataset	Amount	Unit
Inputs			
Casing	Market for steel, low-alloyed	9.79E-01	kg
Casing	Deep drawing, steel	9.79E-01	kg
Sealings	Market for nylon 6	2.11E-02	kg
Infrastructure	Metal working factory construction	4.48E-10	p
Transport lorry	Lorry, >16t, Euro 5, RER	9.79E-02	t·km
Transport train	Market for freight train, EU	1.96E-01	t·km
Outputs			
Cell container	Cell container, 18650 type, for battery	1.00	kg

Electrolyte and separator

The separator is made of polyethylene and is identical to the one used commonly for LIBs [1,14,15]. Thus, the corresponding ecoinvent dataset for battery separator is used [16].

For the electrolyte, a 1 M solution of sodium hexafluorophosphate ($NaPF_6$) in an 80 wt.%-20 wt.% mixture of ethylene carbonate (EC) and dimethyl carbonate (DMC) is used [15,17–19]. This gives, with the densities for EC and DMC [20], an electrolyte composition for a 1.0 M $NaPF_6$ solution according to Table S6.

Table S6. LCI for the production of $NaPF_6$ based electrolyte

Item	Dataset	Amount	Unit
Inputs			
EC (solvent)	Market for ethylene carbonate	7.07E-01	kg
DMC (solvent)	Dimethylcarbonate, from EC, at plant	1.77E-01	kg
NaPF6 (salt)	Sodium hexafluorophosphate, at plant	1.17E-01	kg
Transport, lorry	Lorry, >16t, Euro 5, RER	1.00E-01	t·km
Transport, train	Market for freight train, EU	6.00E-01	t·km
Outputs			
Electrolyte	Electrolyte, $NaPF_6$ based, for Na-Ion battery	1.00	kg

The production of $NaPF_6$ is very similar to that of $LiPF_6$ [21,22]. Thus, the LCI for $NaPF_6$ is derived from the ecoinvent dataset for $LiPF_6$ [23], with slight modifications based on stoichiometric calculations. The corresponding LCI is given in Table S7.

Table S7. LCI for the production of $NaPF_6$

Item	Dataset	Amount	Unit
Inputs			
NaF	Sodium fluoride production	3.19E-01	kg
PCl5	Market for phosphorus pentachloride	1.98	kg
HF	Market for hydrogen fluoride	4.04	kg
Inert atmosphere	Market for nitrogen, liquid	1.25E-03	kg
Neutraliser (lime)	Lime, hydrated, packed, at plant	7.44	kg
Electricity	Medium voltage, market group - EU	5.41E-01	kWh
Transport, lorry	Lorry, >16t, Euro 5, RER	1.38	t·km
Transport, train	Market for freight train, EU	8.27	t·km
Infrastructure	Market for chemical factory, organics	4.00E-10	kg
Outputs			
Disposal of Salts	Disposal, limestone residue, to inert material landfill	8.69	kg
Wastewater	Treatment, sewage, to wastewater treatment	3.61E-03	m3
NaF recycled	Sodium fluoride to recycling	4.24E-02	kg
Emission to air	Phosphorus trichloride, to air	2.63E-01	kg
Waste heat	Heat, waste, to air	1.95	MJ
NaPF6	Sodium hexafluorophosphate, at plant	1.00	kg

DMC can be produced from the reaction of methanol with EC, giving DMC and ethylene glycol [24]. Energy demands for this process are not available, but for the production of DMC from ethylene oxide [4], and the production of EC, the intermediate product, from ethylene oxide [23]. From these two processes, the energy demand of the reaction of EC (which is available in the ecoinvent database) to DMC is derived. Allocation between the two by-products DMC and ethylene glycol is done based on physical relationship (mass). The inventory obtained in this way for DMC production is given in Table S8.

Table S8. LCI for the production of dimethyl carbonate (DMC)

Item	Dataset	Amount	Unit
Inputs			
Ethylene carbonate	Market for ethylene carbonate	9.78E-01	kg
Methanol	Market for methanol	7.11E-01	kg
Electricity	Medium voltage, market group - EU	2.63E-03	kWh
Heat	Central or small scale, natural gas - EU	1.01E-01	MJ
Infrastructure	Market for chemical factory, organics	6.76E-10	p
Outputs			
DMC (solvent)	Dimethylcarbonate, from EC, at plant	1.00	kg
Ethylene glycol	Ethylene glycol, from DMC production, at plant	6.89E-01	kg

Cathode production

For casting the cathode, the active material is mixed with carbon black, a PVdF copolymer binder and N-methyl-2-pyrrolidone (NMP) as solvent in a ball mill, obtaining an electrode slurry with a solid content of 65%, which is the cast onto the substrate (current collector foil) [8,9,25,26]. Energy requirements for slurry mixing and casting are derived from Notter et al. [8], while the heat demand is calculated based on the heat capacity and the enthalpy of evaporation for the NMP solvent, assuming an 80% efficient dryer [27]. Furthermore, an internal solvent (NMP) recovery of 99% is freely assumed, with the remaining 1% being accounted for as emissions to air. For transport services, the standard ecoinvent distances for inorganic chemicals are used. The inventory obtained in this way is given in Table S9.

Table S9. LCI for the production of a cathode

Item	Dataset	Amount	Unit
Inputs			
Active material	NMMT active material, layered oxide, for Na-Ion bat.	8.54E-01	kg
Carbon black	Market for carbon black	1.82E-02	kg
PvDF binder	Market for tetrafluoroethylene	1.82E-02	kg
PvDF binder	Market for polyethylene, low density	1.82E-02	kg
NMP solvent	Market for N-methyl-2-pyrrolidone	3.18E-03	kg
Electricity	Medium voltage, market group - EU	2.00E-03	kWh
Heat	Central or small scale, natural gas - EU	2.67E-01	MJ
Substrate (Al foil)	Aluminium, wrought alloy	9.11E-02	kg
Substrate (Al foil)	Sheet rolling, aluminium	9.11E-02	kg
Transport lorry	Lorry, >16t, Euro 5, RER	1.49E-02	t·km
Transport train	Market for freight train, EU	5.28E-02	t·km
Infrastructure	Metal working factory construction	4.58E-10	p
Outputs			
NMP emission	1-Methyl-2-pyrrolidinone, to air	3.18E-03	kg
Waste heat	Heat, waste, to air	2.67E-01	MJ
Cathode	Cathode, NMMT layered oxide, for Na-Ion battery	1.00	kg

Cathode active material production ($Na_{1.1}Ni_{0.3}Mn_{0.5}Mg_{0.05}Ti_{0.05}O_2$ - NMMT layered oxide)

The active material used for the Na-Ion battery is a layered oxide, $Na_{1.1}Ni_{0.3}Mn_{0.5}Mg_{0.05}Ti_{0.05}O_2$ [25]. For its production, the precursor materials (sodium carbonate, manganese oxide, nickel carbonate, magnesium hydroxide and titanium dioxide) are intimately ball milled together and pressed into pellets. These are then heated in a furnace and maintained at 900°C for 8 hours. After cooling down, the product is milled and used for producing the cathode slurry [25,28]. Electricity demand for driving the rotary kiln and for ball milling are taken from reference processes (rotary kiln for titanium dioxide production [27] and cathode slurry preparation in ball mill [8], respectively). The heat demand is estimated based on the heat capacity of the materials [29] and a kiln efficiency of 10%, what is comparably low [30], but tries to account for the long residence time and the omission of the reaction enthalpy. This gives a heat demand well in between the 15 MJ obtained by Notter et al. [8] and the 3 MJ of the reference process, a rotary kiln in titanium dioxide production that operates at the same temperature, but with significantly shorter residence times [27]. For the precursor materials TiO_2, Na_2CO_3 and MnO_2, the ecoinvent datasets are used [23], while the production of

$NiCO_3$ and $Mg(OH)_2$ has to be modelled explicitly. Table S10 presents the LCI data for the active material production.

Table S10. LCI for the production of NMMT active cathode material

Item	Dataset	Amount	Unit
Inputs			
Na_2CO_3	Market for soda ash, dense	5.50E-01	kg
MnO_2	Market for manganese dioxide	4.10E-01	kg
$NiCO_3$	Nickel carbonate, anhydrous, at plant	3.36E-01	kg
$Mg(OH)_2$	Magnesium hydroxide, at plant	2.75E-02	kg
TiO_2	Market for titanium dioxide	3.77E-02	kg
Electricity	Medium voltage, market group - EU	3.08E-02	kWh
Heat	Central or small scale, natural gas - EU	10.60	MJ
Transport, lorry	Lorry, >16t, Euro 5, RER	1.36E-01	t·km
Transport, train	Market for freight train, EU	8.17E-01	t·km
Infrastructure	Market for chemical factory, organics	4.00E-10	p
Outputs			
CO_2	Carbon dioxide, fossil, to air	3.53E-01	kg
Waste heat	Heat, waste, to air	10.71	kg
Active material	NMMT active material, layered oxide, for Na-Ion bat.	1.00	kg

Magnesium hydroxide ($Mg(OH)_2$) production

Magnesium hydroxide is commonly obtained as milk of magnesia in a simple process from seawater brines, where Mg is contained in sufficient concentration (1.2-1.3 $g \cdot l^{-1}$ in average) [31]. Concentrated brine is mixed with hydrated lime, what leads to the formation of $Mg(OH)_2$, which precipitates as a suspension (“milk of magnesia”) that can be separated from the brine by centrifugation and / or filtering [32].

The brine is assumed to be concentrated in open ponds by sunlight, why no further energy is required. The energy required for brine handling and pumping is derived from the ecoinvent process “Li brine inspissation” [8,33], what is considered a valid proxy since the concentration of Mg in seawater is comparable to that of Li in lithium brine lakes. In contrast to the lithium brines, seawater brine is assumed to be produced in sites with electricity grid availability, so the required diesel fuel is converted to electricity by dividing by factor 3. The electricity required by the stirring reactor is taken from a comparable reference process (Salt dissolver from an alkaline and chlorine production process [27]). A 20% overliming, 95% conversion efficiency and 98% $Mg(OH)_2$ recovery efficiency is further assumed. The inventory obtained in this way is given in Table S11.

Table S11. LCI for the production of $Mg(OH)_2$

Item	Dataset	Amount	Unit
Inputs			
Brine	Sodium chloride, brine solution, market - GLO	105.79	kg
Hydrated lime	Lime, hydrated, loose, market	1.20	kg
Electricity	Medium voltage, market group - EU	1.78	kWh
Transformation	Unknown to mineral extracting site	3.26E-02	m2
Occupation	Mineral extraction site	1.63	m2a
Transport, lorry	Lorry, >16t, Euro 5, RER	1.20E-01	t·km
Transport, rail	Market for freight train, EU	7.17E-01	t·km
Outputs			
Heat, waste	Heat, waste, to air	6.42	MJ
$Mg(OH)_2$	Magnesium hydroxide, at plant	1.00	kg

Nickel carbonate ($NiCO_3$) preparation

Commercial basic nickel carbonate is made by precipitation from a nickel solution, usually the sulphate, with sodium carbonate, being the exact reaction mechanism $NiSO_4 + 2 NaHCO_3 \rightarrow NiCO_3 + Na_2SO_4 + H_20 + CO_2$ [34]. Details about the process required for modelling are derived from patents [35,36]: The Sodium hydrogen carbonate reacts at 50°C with a nickel chloride solution that has a nickel concentration of 177 $g \cdot l^{-1}$, obtaining a wet precipitate with a nickel content of about 27.5% and carbon dioxide. Centrifugation and hot air drying produces anhydrous $NiCO_3$ with a final Ni content of 49.3%. The electricity demand is derived from reference processes (pumping, centrifugation and filtration from a titanium dioxide production process, and the operation of the stirring reactor from an alkaline and chlorine production process [27]). The heat demand for heating the reactor and for drying the $NiCO_3$ precipitate is calculated based on the latent heat of the materials [20,29] and the heat for evaporation of water, assuming an average 5% heat losses to the environment from the stirred tank reactor, and a gross efficiency of the dryer of 80% [27]. Since no inventory data for $NaHCO_3$ can be found in the ecoinvent database, soda ash is used instead. $NaHCO_3$ is an intermediate product of soda ash production (soda ash is obtained in the end of the process by heating $NaHCO_3$, obtaining Na_2CO_3)[23]. Accounting soda ash instead of sodium hydrogen carbonate thus overestimates the impacts of $NaHCO_3$ production slightly and can be considered a conservative assumption. No further wastewater treatment is assumed for the process. Table S12 gives the corresponding LCI.

Table S12. LCI for the production of $NiCO_3$

Item	Dataset	Amount	Unit
Inputs			
$NaHCO_3$	Market for soda ash, dense	1.42	kg
$NiSO_4$	Nickel sulphate production	1.30	kg
Water	Water, deionised, from tap water	7.98	kg
Electricity	Medium voltage, market group - EU	1.12E-02	kWh
Heat	Central or small scale, natural gas - EU	2.62	MJ
Transport, lorry	Lorry, >16t, Euro 5, RER	2.72E-01	t·km
Transport, rail	Market for freight train, EU	1.63	t·km
Outputs			
CO_2	Carbon dioxide, fossil, to air	3.71E-01	kg
Na_2SO_4 in effluent	Sodium, ion, to river	1.94E-01	kg
Na_2SO_4 in effluent	Sulfate, to river	8.09E-01	kg
$NiCO_3$ in effluent	Nickel, ion, to river	1.27E-02	kg
$NiCO_3$ in effluent	Carbonate, to river	1.30E-02	kg
Waste heat	Heat, waste, to air	2.29	MJ
$NiCO_3$	Nickel carbonate, anhydrous, at plant	1.00	kg

Anode production

Similar as for the cathode, the negative electrode is prepared by solvent-casting of a slurry of hard carbon active material, conductive carbon, binder and solvent [8,25,26]. For the anode, a water based binder is used, a 70:30 mixture of carboxymethyl-cellulose (CMC) and styrene-butadiene rubber (SBR) [6,7]. Around 40 g of water are used as solvent per 100 g of anode material (slurry solid content 60%). Efficiencies and energy requirements for milling, casting and solvent evaporation at 100°C are estimated like for the cathode production process based on the enthalpy of evaporation and the heat capacity of the solvent (water). Like for the cathode, it is assumed that the hard carbon material is synthesized at the plant where anode is prepared and thus no transport of active material is required. The inventory obtained for the production of 1 kg of anode is given in Table S13.

SBR production

SBR is not contained in ecoinvent and its production needs to be modelled explicitly. SBR is produced from styrene and butadiene in a continuous polymerisation process: Butadiene and styrene are mixed in an aqueous medium by the help of a surfactant / emulsifier (soap or tensides). An initiator (e.g. persulfate) starts the radical the polymerisation process [37–39]. Heat and electricity demand, and the corresponding emissions from are derived from generic industrial process data for SBR production processes [40–42]. As surfactant, soap is assumed (the choice of the surfactant is of little influence; alkylbenzene sulfonate as alternative shows very similar results). The corresponding inventory data can be retrieved from Table S14.

Table S13. LCI for the production of a hard carbon anode with aqueous binder

Item	Dataset	Amount	Unit
Inputs			
Hard carbon	Hard carbon, anode, from sugar	8.01E-01	kg
Carbon black	Market for carbon black	2.59E-02	kg
CMC (binder)	Market for carboxymethyl cellulose, powder	2.42E-02	kg
SBR (binder)	Styrene- butadiene rubber (SBR)	1.04E-02	kg
Water (solvent)	Market for water, deionised, from tap water	3.45E-01	kg
Electricity	Medium voltage, market group - EU	2.06E-06	kWh
Heat	Central or small scale, natural gas - EU	1.11	MJ
Substrate (Al foil)	Market for aluminium, wrought alloy	1.38E-01	kg
Substrate (Al foil)	Market for sheet rolling, aluminium	1.38E-01	kg
Transport, lorry	Lorry, >16t, Euro 5, RER	1.88E-02	t·km
Transport, train	Market for freight train, EU	5.77E-02	t·km
Infrastructure	Metal working factory construction	4.58E-10	p
Outputs			
Water	Water, to air	3.45E-01	kg
Waste heat	Heat, waste, to air	1.12	MJ
Anode (water based binder)	Anode, hard carbon-Al, for Na-Ion battery	1.00	kg

Table S14. LCI for the production of styrene butadiene rubber (SBR)

Item	Dataset	Amount	Unit
Inputs			
Butadiene	Market for butadiene	7.52E-01	kg
Styrene	Market for styrene	2.51E-01	kg
Emulsifier	Market for soap	2.73E-02	kg
Water	Market for water, deionised, from tap water	1.80	kg
Solvent make up	Cyclohexane production	1.00E-02	kg
Initiator (persulfate)	Market for sodium persulfate	5.04E-03	kg
Electricity	Medium voltage, market group - EU	5.50E-01	kWh
Heat	Central or small scale, natural gas - EU	13.75	MJ
Cooling water	Water, cooling, unspecified natural origin	2.50E-01	m3
Infrastructure	Market for chemical factory, organics	4.00E-10	p
Transport, lorry	Lorry, >16t, Euro 5, RER	1.05E-01	t·km
Transport, train	Market for freight train, EU	6.27E-01	t·km
Outputs			
NMVOC	NMVOC, unspecified origin	1.44E-02	kg
Waste heat	Heat, waste, to air	15.73	MJ
Wastewater	Treatment of wastewater, unpolluted	1.80	kg
SBR	Styrene- butadiene rubber (SBR)	1.00	kg

Hard carbon (anode active material) production

For hard carbon synthesis, a carbohydrate precursor is treated thermally in a first stage under ambient atmosphere at 300°C, obtaining a dry degraded carbohydrate. In a second stage, the brittle product is milled and then subjected to calcination under inert (nitrogen) atmosphere for three hours at around 1100°C, obtaining hard carbon. The hard carbon pellets are milled for their use as active material in the anode preparation process [1]. No further information is given about the used carbohydrate precursor, why it is assumed to be sugar, readily available in industrial amounts with constant quality on the market. The energy demand, emissions and waste streams of the first heating step are derived entirely from technical data about wood torrefaction plants, since the reaction conditions are comparable those of a biomass torrefaction process [43]. The torrefaction plant also consumes a certain amount of no further specified additives, which are accounted for as unspecific organic chemicals. For the second stage, the final calcination, it is assumed that the hard carbon yield from sugar is equivalent the fixed carbon content of cellulose (a sugar polymer), which is around 11% [44]. Emissions are then calculated based on stoichiometric considerations, assuming a carbon content for sugar of 42% [44] and 99% for hard carbon. The amount of nitrogen for maintaining the inert atmosphere is derived from a reference process, $MnCO_3$ roasting under inert atmosphere in rotary kiln [8]. The heat demand for the calcination kiln is then estimated based on the specific heat capacities of the nitrogen gas and the torrefied sugar feed, assuming an average 12.5% heat losses to the environment from the rotary kiln [27]. Electricity demand is obtained from the electricity consumption of the torrefaction plant [43] plus the energy required for milling of torrefied wood pellets [45]. The transport distances for the carbohydrate precursors are calculated using the standard transport distances from ecoinvent for wood products as proxy. The LCI obtained in this way for the hard carbon synthesis process is given in Table S15.

Table S15. LCI for the production of hard carbon from sugar precursor

Item	Dataset	Amount	Unit
Inputs			
Carbohydrate	Market for sugar, from sugar beet	20.00	kg
Electricity	Medium voltage, market group - EU	1.07E-01	kWh
Heat	Central or small scale, natural gas - EU	9.52	MJ
Water	Market for water, deionised, from tap water	1.78E-01	l
Additives	Market for chemicals, inorganic	2.67E-01	kg
Inert atmosphere	Market for nitrogen, liquid	6.99	kg
Transport, lorry	Lorry, >16t, Euro 5, RER	1.38	t·km
Transport, train	Market for freight train, EU	4.86	t·km
Infrastructure	Market for chemical factory, organics	4.00E-10	p
Outputs			
Dust	Dust, unspecified, to air	6.62E-05	kg
CO_2	Carbon dioxide, biogenic, to air	29.33	kg
CO	Carbon monoxide, biogenic, to air	3.53E-04	kg
NO_x	Nitrogen oxides, to air	6.16E-03	kg
SO_2	Sulphur dioxide, to air	1.17E-03	kg
TOC	NMVOC, to air	1.10E-04	kg
HF	Hydrogen fluoride, to air	8.89E-06	kg
HCl	Hydrogen chloride, to air	5.08E-04	kg
Waste heat	Heat, waste, to air	9.90	MJ
Waste water	Treatment of wastewater, average	1.78E-02	l
Solid waste	Market for municipal solid waste	4.44E-04	kg
Hard carbon	Hard carbon, anode, from sugar	1.00	kg

Alternatively, hard carbon can be produced from fossil precursors like petroleum coke [46,47]. For the sensitivity analysis, this process is modelled explicitly, since petroleum coke differs fundamentally from organic carbohydrates and thus the use of the same LCI is considered to be inadequate. Green petroleum coke is calcined in a rotary kiln under protective atmosphere at temperatures around 1100°C. The process is similar to the calcination of the torrefied carbohydrate, but yields and energy demands vary fundamentally [48,49]. These are estimated based on stoichiometric calculations for a green petroleum coke with an overall carbon content of 89% and a fixed carbon content of roughly 2 percent points lower [50–53]. The obtained hard carbon is assumed to be identical to the one from organic precursors (99% carbon content). Kiln residence times and heat loss is assumed to be identical in both cases, but due to the higher yield of hard carbon from petroleum coke, the amount of required feedstock and thus the kiln volume is significantly lower, reducing the energy demand of the process. For coke, standard transport distances for petroleum products are used according to ecoinvent. Table S16 provides the LCI for the production of hard carbon from petroleum coke, as used for the sensitivity analysis.

Table S16. LCI for the production of hard carbon from petroleum coke

Item	Dataset	Amount	Unit
Inputs			
Coke	Market for petroleum coke	1.14	kg
Electricity	Medium voltage, market group - EU	1.83E-02	kWh
Heat	Central or small scale, natural gas - EU	1.89	MJ
Water	Market for water, deionised, from tap water	1.78E-01	l
Inert atmosphere	Market for nitrogen, liquid	9.00E-01	kg
Transport, lorry	Lorry, >16t, Euro 5, RER	1.59E-01	t·km
Transport, train	Market for freight train, EU	7.77E-01	t·km
Infrastructure	Market for chemical factory, organics	4.00E-10	p
Outputs			
CO_2	Carbon dioxide, fossil, to air	8.39E-02	kg
NO	Nitrogen oxide, to air	4.66E-02	kg
NO_2	Nitrogen dioxide, to air	3.76E-03	kg
SO_2	Sulphur dioxide, to air	5.03E-02	kg
Waste heat	Heat, waste, to air	1.95	MJ
Hard carbon	Hard carbon, anode, from petroleum coke	1.00	kg

Impact assessment methodology (LCIA)

The impact categories considered for assessment in the paper are explained briefly in the following:

- **FDP** (fossil depletion potential): Depletion of fossil energy resources (e.g. ‘peak oil’), measured in kg of oil equivalent.
- **GWP** (global warming potential): Emission of greenhouse gases like CO_2, methane, N_2O, etc. (‘global warming’). Measured in kg of CO_2 equivalents.
- **TAP** (terrestrial acidification potential): Emission of acidifying substances (SO_2, NO_x, etc.) that change the pH of soil and water and thus put pressure on the ecosystem (‘acid rain’). Measured in kg of SO_2 equivalents
- **MEP** and **FEP** (marine and freshwater eutrophication): deposition of macronutrients (nitrogen and phosphorous) in groundwater and watercourses, leading to change in the natural equilibrium, uncontrolled algae growth and oxygen depletion (dying water bodies / ‘dead zones’). Measured in kg of N and P equivalents, respectively.

Being these the most commonly assessed impact categories, the ReCiPe methodology quantifies other ones that are not discussed in detail in the paper. Nevertheless, the results for these categories might be of interest to certain readers and are tabulated additionally in the SI, but not explained further. Presenting and discussing them all in the main paper would widen the scope too much and make the paper difficult to read.

The impact category MDP (metal depletion) has to be mentioned explicitly, since it can be considered of special interest for the assessment of SIBs, being the use of abundant raw materials one of the arguments in favour of them. Nevertheless, it turned out that the ReCiPe methodology shows an extraordinarily high metal depletion impact for manganese, a comparably abundant material, also in comparison to other common impact assessment categories. This produces extremely unfavourable results for all manganese containing batteries (LMO-C, NCM-C, and also the assessed SIB). In fact, for the assessed SIB, the use of the manganese for the cathode alone contributes to 64% of the overall MDP impact, while the nickel demand from the $NiCO_3$ precursor is responsible for only 11.5%, being nickel less abundant than manganese. LMO-C LIBs also score significantly worse than other LIB types that use much more scarce metal precursors like NCA-C. Another shortcoming of the ReCiPe impact assessment methodology is that lithium has no characterization factor for the MDP category and thus the consumption of lithium does not contribute in any way to the obtained impact of LIBs. This is evidently not true, and one of the advantages of SIBs, the substitution of lithium by more abundant sodium, is not reflected in the results. Nevertheless, compared to the high contribution of manganese, this effect can be expected to be rather small, being the depletion of lithium in general only a small fraction in the environmental impacts of LIB production [26,54–56]. In any case, the methodology is considered to be unsuitable for comparing manganese containing batteries under metal depletion aspects and the MDP results are therefore not discussed further. They are nevertheless included in the corresponding Tables in the following.

Comparison with LIB

For comparing the environmental performance of SIB with current LIBs, it is contrasted with existing LCA studies on LIBs. Nevertheless, significant discrepancies exist also in the modelling of the LCI between these studies, making a direct comparison difficult. One of the main discrepancies is the approach for modelling the energy demand during cell and battery pack manufacturing, which affects the results significantly, while varying up to an order of magnitude [5,13,26]. In order to reduce these discrepancies, the LCI of the different studies are recompiled using a common average value and the same European electricity mix. The average electricity demand for cell and pack manufacturing obtained from the studies is 6.44 kWh, and the heat demand 21.01 MJ. Still, some important differences exist in the modelling approaches of the different studies (type of electrode binder, BMS), why direct comparison of results from different studies has to be done with care. The characterisation results obtained per kWh of storage capacity for the different batteries are given in Table S17.

Table S17. Characterization values for the compared batteries (per kWh of storage capacity) . GWP = global warming potential, FDP = fossil depletion potential, MDP = metal depletion potential, MEP = marine eutrophication potential, FEP = freshwater eutrophication potential, HTP = human toxicity potential, TAP = terrestrial acidification potential, ODP = ozone depletion potential, PMP = particulate matter formation, POF = photochemical oxidant formation, TETP = terrestrial ecotoxicity potential, METP = marine ecotoxicity potential, FETP = freshwater ecotoxicity potential

Category	Unit	LFP-C (M-B)	LFP-C (Zak)	LFP-LTO (Bau)	LMO-C (Not)	NCA-C (Bau)	NCM-C (M-B)	Na-Ion
GWP	kg CO_2-Eq	267.42	200.14	255.99	111.94	110.78	209.71	140.31
FDP	kg oil-Eq	54.60	41.99	72.01	33.51	30.69	43.19	37.33
MDP	kg Fe-Eq	71.31	259.52	36.97	166.53	67.48	120.35	104.99
MEP	kg N-Eq	2.25E-01	2.14E-01	2.26E-01	1.44E-01	1.31E-01	1.89E-01	3.05E-01
FEP	kg P-Eq	3.78E-01	4.51E-01	2.00E-01	2.04E-01	1.64E-01	2.88E-01	1.20E-01
HTP	kg 1,4-DCB-Eq	576.99	769.14	251.94	369.98	275.57	478.11	168.20
TAP	kg SO_2-Eq	1.22	2.23	1.18	0.96	2.62	2.13	1.51
ODP	kg CFC-11-Eq	2.58E-03	2.26E-03	1.15E-03	9.66E-06	2.72E-04	1.95E-03	3.73E-04
PMF	kg PM10-Eq	5.20E-01	5.69E-01	4.76E-01	3.82E-01	6.65E-01	6.63E-01	4.57E-01
POF	kg NMVOC	5.99E-01	5.40E-01	6.31E-01	4.04E-01	5.04E-01	6.02E-01	4.70E-01
TETP	kg 1,4-DCB-Eq	2.41E-02	2.17E-02	1.80E-02	2.33E-02	2.22E-02	2.13E-02	1.90E-02
METP	kg 1,4-DCB-Eq	11.28	14.41	6.16	7.42	5.86	9.84	4.31

FETP	kg 1,4-DCB-Eq	11.74	14.95	6.60	7.37	5.82	10.19	4.55

Sensitivity Analysis

Different hard carbon precursors

For the sensitivity analysis, the amount of sugar is substituted by the equal amount of the alternative organic carbohydrate material (starch, cellulose and organic residues). Starch and cellulose are taken directly from ecoinvent, while for organic residues a generic residue is assumed as representative for organic waste materials like fruit peels or apple waste [57,58]. According to the cut-off system model of ecoinvent 3.2., the waste is available free of burden and no bonus for potentially avoided waste treatment or by-products from the waste treatment is accounted for. Since all are carbohydrates with similar carbon content, it is further assumed that the remaining process conditions and yields do not change. This is certainly a simplification, especially if precursors with higher water content are used, but since the process itself has comparably little influence in comparison with the precursor production, it is considered valid for the sensitivity analysis. For evaluating petroleum coke as alternative (fossil) precursor for hard carbon production, the corresponding LCI as given in Table S16 is used. The obtained results are tabulated in Table S18. Comparably good results are obtained for the petroleum coke, basically due to the high assumed yields. Since no data on hard carbon yields from petroleum coke is available, these are estimated based on the fixed carbon content of the materials.

Table S18. Characterization values for the different SIB hard carbon precursors (per kWh of storage capacity). Abbreviations of impact categories as in Table S17.

Category	Unit	Sugar	Starch	Cellulose	Org. waste	Petr. coke
GWP	kg CO_2-Eq	140.31	150.84	143.56	117.06	110.91
FDP	kg oil-Eq	37.33	39.79	40.12	31.46	29.94
MDP	kg Fe-Eq	104.99	109.01	107.54	104.04	103.87
MEP	kg N-Eq	3.05E-01	4.53E-01	1.58E-01	1.14E-01	1.03E-01
FEP	kg P-Eq	1.20E-01	1.28E-01	1.25E-01	1.13E-01	1.10E-01
HTP	kg 1,4-DCB-Eq	168.20	182.74	182.04	164.14	161.17
TAP	kg SO_2-Eq	1.51	1.70	1.50	1.32	1.40
ODP	kg CFC-11-Eq	3.73E-04	3.74E-04	3.74E-04	3.71E-04	3.71E-04
PMF	kg PM10-Eq	4.57E-01	5.02E-01	5.04E-01	3.95E-01	4.06E-01
POF	kg NMVOC	4.70E-01	5.16E-01	5.12E-01	3.81E-01	3.60E-01
TETP	kg 1,4-DCB-Eq	1.90E-02	9.18E-02	1.88E-02	1.53E-02	1.44E-02
METP	kg 1,4-DCB-Eq	4.31	4.88	4.97	4.12	4.02
FETP	kg 1,4-DCB-Eq	4.55	5.14	5.22	4.28	4.18

Battery internal efficiency

The characterization values obtained for the storage of 1 kWh of electricity over battery lifetime are shown in Table S19. An average 80% depth of discharge (DoD) is assumed in each charge/discharge cycle, and a European electricity mix is used for this estimation[59].

Table S19. Variation of the environmental impacts per kWh of electricity stored over battery lifetime with battery internal efficiency. Abbreviations of impact categories as in Table S17.

Category	Unit	85%	90%	95%
GWP	kg CO_2-Eq	1.59E-01	1.35E-01	1.12E-01
FDP	kg oil-Eq	4.28E-02	3.63E-02	2.98E-02
MDP	kg Fe-Eq	6.66E-02	6.63E-02	6.59E-02
MEP	kg N-Eq	2.49E-04	2.30E-04	2.10E-04
FEP	kg P-Eq	1.38E-04	1.17E-04	9.58E-05
HTP	kg 1,4-DCB-Eq	1.48E-01	1.34E-01	1.19E-01
TAP	kg SO_2-Eq	1.24E-03	1.14E-03	1.04E-03
ODP	kg CFC-11-Eq	2.40E-07	2.38E-07	2.36E-07
PMF	kg PM10-Eq	3.82E-04	3.50E-04	3.18E-04
POF	kg NMVOC	4.36E-04	3.89E-04	3.41E-04
TETP	kg 1,4-DCB-Eq	1.40E-05	1.33E-05	1.26E-05
METP	kg 1,4-DCB-Eq	4.07E-03	3.61E-03	3.15E-03
FETP	kg 1,4-DCB-Eq	4.31E-03	3.82E-03	3.33E-03

Different binder for electrodes

For casting the anode and cathode electrodes, a binder is needed in combination with the adequate solvent. For the assessed SIB, it is assumed according to the current state of the art that for the anode, a water based binder is used (CMC-SBR), while the cathode uses an organic solvent (NMP and PVdF as binder). In order to evaluate the influence of the binder / solvent on the overall results, we calculate two alternative configurations, an all- water based battery (water/CMC-SBR both for anode and cathode) and an all-organic battery (NMP/PVdF for both electrodes). The LCI for the alternative electrode production processes (anode with organic binder, cathode with water based binder) are calculated like previously described for the anode and cathode production process: Around 40 g of water are used as solvent per 100 g of water based cathode material, and 35 g NMP per 100 g of organic anode material. Energy requirements are adjusted according to the different amounts, heat capacities and evaporation enthalpies of the solvents. The LCI obtained in this way for the organic solvent based anode and the water solvent based cathode are given in Tables S20 and S21, respectively. Table S22 then contains the characterization results obtained for these two alternative battery configurations (all water based electrodes / base case – organic cathode and water based anode / all organic solvent based electrodes). As can be observed, the binder affects above all the

GWP (8.6% reduction for all-water-based binder compared to base case) and the ODP (improvement of almost one order of magnitude), while it changes relatively little in the remaining categories.

Table S20. LCI for the production of a cathode with water based binder

Item	Dataset	Amount	Unit
Inputs			
Active material	NMMT active material, layered oxide, for Na-Ion bat.	8.54E-01	kg
Carbon black	Market for carbon black	1.82E-02	kg
CMC (binder)	Market for carboxymethyl cellulose, powder	2.54E-02	kg
SBR (binder)		1.09E-02	kg
Water	Market for water, deionised, from tap water	3.64E-01	kg
Electricity	Medium voltage, market group - EU	2.07E-03	kWh
Heat	Central or small scale, natural gas - EU	1.17	MJ
Substrate (Al foil)	Aluminium, wrought alloy	9.11E-02	kg
Substrate (Al foil)	Sheet rolling, aluminium	9.11E-02	kg
Transport lorry	Lorry, >16t, Euro 5, RER	1.35E-02	t·km
Transport train	Market for freight train, EU	4.44E-02	t·km
Infrastructure	Metal working factory construction	4.58E-10	p
Outputs			
Water	Water, to air	3.64E-01	kg
Waste heat	Heat, waste, to air	1.18	MJ
Cathode, water based	Cathode, NMMT layered oxide, for Na-Ion battery	1.00	kg

Table S21. LCI for the production of an anode with organic solvent based binder

Item	Dataset	Amount	Unit
Inputs			
Hard carbon	Hard carbon, anode, from sugar	8.01E-01	kg
Carbon black	Market for carbon black	2.59E-02	kg
PvDF binder	Market for tetrafluoroethylene	1.73E-02	kg
PvDF binder	Market for polyethylene, low density	1.73E-02	kg
NMP solvent	Market for N-methyl-2-pyrrolidone	3.02E-02	kg
Electricity	Medium voltage, market group - EU	2.00E-03	kWh
Heat	Central or small scale, natural gas - EU	2.53E-01	MJ
Substrate (Al foil)	Market for aluminium, wrought alloy	1.38E-01	kg
Substrate (Al foil)	Market for sheet rolling, aluminium	1.38E-01	kg
Transport, lorry	Lorry, >16t, Euro 5, RER	2.29E-02	t·km
Transport, train	Market for freight train, EU	8.20E-02	t·km
Infrastructure	Metal working factory construction	4.58E-10	p
Outputs			
NMP	1-Methyl-2-pyrrolidone, to air	3.02E-02	kg
Waste heat	Heat, waste, to air	2.53E-01	MJ
Anode, organic binder	Anode, hard carbon-Al, for Na-Ion battery	1.00	kg

Table S22. Environmental impacts obtained for the SIB with different electrode binder in each category (per kWh of storage capacity). All water = cathode and anode with water based binder (CMC); base case = cathode with organic (PVdF) and anode with water based binder; all organic = cathode and anode with water based binder. Other abbreviations (impact categories) as in Table S17.

Category	Unit	all water	base case	all organic
GWP	kg CO_2-Eq	128.32	140.31	156.23
FDP	kg oil-Eq	37.26	37.33	37.59
MDP	kg Fe-Eq	104.96	104.99	105.05
MEP	kg N-Eq	3.05E-01	3.05E-01	3.06E-01
FEP	kg P-Eq	1.20E-01	1.20E-01	1.20E-01
HTP	kg 1,4-DCB-Eq	167.30	168.20	169.63
TAP	kg SO_2-Eq	1.51	1.51	1.52
ODP	kg CFC-11-Eq	1.09E-05	3.73E-04	8.36E-04
PMF	kg PM10-Eq	4.57E-01	4.57E-01	4.59E-01
POF	kg NMVOC	4.69E-01	4.70E-01	4.73E-01
TETP	kg 1,4-DCB-Eq	1.89E-02	1.90E-02	1.89E-02
METP	kg 1,4-DCB-Eq	4.31	4.31	4.33
FETP	kg 1,4-DCB-Eq	4.54	4.55	4.56

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