Life Cycle Assessment of Stationary Storage Systems within the Italian Electric Network

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Summary: These Supplementary Materials contain a full inventory of the different battery components.

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1 SYSTEM DESCRIPTION: BATTERY PRODUCTION AND ASSEMBLY

For the definition of the battery production and assembly phase, we referred to the diagram published by Ellingsen et al. [1] (Figure S1), and battery component composition is summarized in Figure S2.

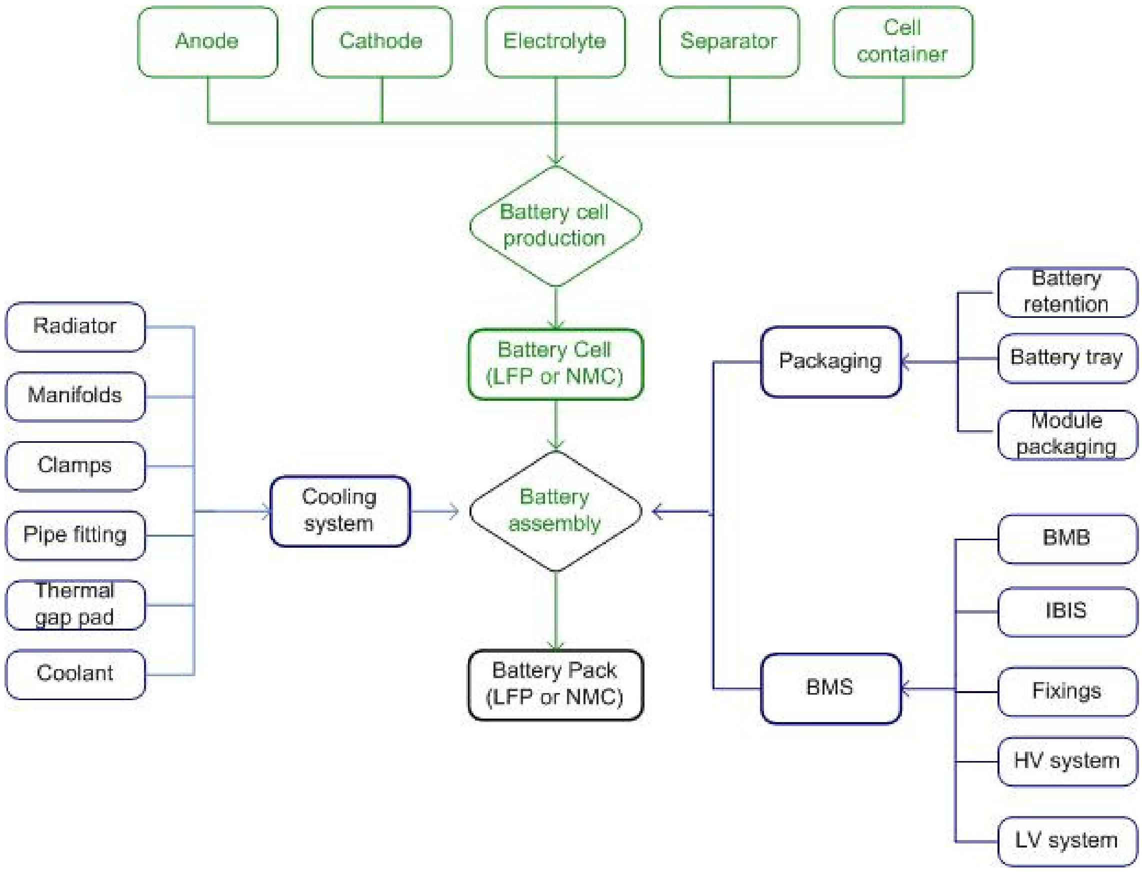

Figure S1. General flowchart of the batteries, adapted from [1] (BMS: battery management system, MBM: battery management board; IBIS: integrated battery interface system, HV: high voltage; LV: low voltage)

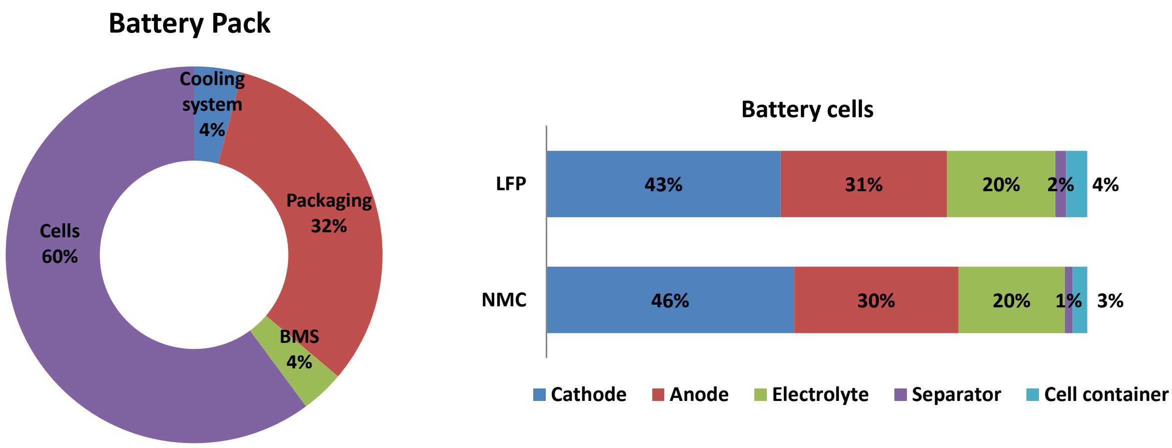

Figure S2. Battery pack and battery cell mass composition, by components

2 LIFE CYCLE INVENTORY (LCI)

The inventory analysis includes data collection and calculation procedures to quantify the relevant inputs and outputs of the analyzed system. The process is iterative: after collecting the data and starting to better understand the characteristics of the system, new needs and limitations of the owned elements should be identified.

Data collection includes data validation and identifying data's relationship with the process units, reference flow, and functional unit. These operations are necessary to provide the results of the inventory phase for each process unit and for the overall functional unit.
Data can be of two types: primary (coming from direct surveys) or secondary (taken from existing literature). In the following paragraphs, the inventory analysis of all the battery components is carried out, considering the storage systems three main life cycle phases: production and assembly, use phase, and end-of-life (EoL).

2.1 Production phase

2.1.1 Battery Pack

The battery mass composition, presented in Figure S2, was determined by combining primary data, for the different battery cells, provided by an Italian producer of storage systems and the information reported by Ellingsen et al. [1]. The analyzed batteries have a capacity of 26.6 kWh, as the one reported by [1].
The lithium–iron–phosphate (LFP) battery has a total mass of 335 kg, while the mass of nickel–manganese–cobalt (NMC) 532 and NMC 622 was 314 kg.

Energy consumption related to the battery assembly phase was modelled by the medium voltage Italian electricity mix, as defined by [2].

Table S1 summarizes the information contained within the datasets relating to the production phase of 1 kg of the LFP, NMC 532, and NMC 622 batteries.

Table S1. Dataset for the production of 1 kg of battery: LFP, NMC 532, and NMC 622. The source of information used is mentioned in the name

Dataset	Amount	Units
UF Output		
Li-ion battery production_1 Kg of battery pack LFP or NMC 532 or NMC 622	1.00E+00	kg
Materials/Fuels Input		
Transport, freight, lorry 7.5–16 metric ton, EURO5 {RER}∣ transport, freight, lorry 7.5–16 metric ton, EURO5 ∣ Alloc Rec, U	5.00E-03	tkm
Precious metal refinery {SE}∣ construction ∣ Alloc Rec, U	1.90E-08	p
Li-ion battery production_cooling system ∣ Alloc Rec, U_Ellingsen_2013_RSE	4.10E-02	kg
LFP: Li-ion battery cell production_LFP ∣ Alloc Rec, U _RSE NMC 532: Li-ion battery cell production_NMC 532 ∣ Alloc Rec, U_RSE NMC 622: Li-ion battery cell production_NMC 532 ∣ Alloc Rec, U_RSE	6.00E-01	kg
Li-ion battery production_Packaging ∣ Alloc Rec, U_Ellingsen_2013_RSE	3.20E-01	kg
Li-ion battery production_BMS ∣ Alloc Rec, U_Ellingsen_2013_RSE	3.70E-02	kg
Electricity/Heat		
Electricity, medium voltage {IT}∣ Electricity Production mix∣ Alloc Rec, U_RSE	4.00E-04	kWh
Emissions		
Heat and waste	1.40E-03	MJ

2.1.2 Battery Cells

As reported in Figure S2, cells are responsible for 60% of battery weight. Each cell consists of five main elements: the anode, cathode, electrolyte, separator, and cell container. Considering cell production in Italy, the Italian energy mix (the same considered for battery assembly) was used in this study. Figure S2. summarizes the information contained within the dataset related to the production of 1 kg of LFP battery cells, and Table S3. Dataset summarizes the information contained within the dataset related to the production of 1 kg of NMC 532 and NMC 622 battery cells.

The Ecoinvent data set: Polyol {RER} | production | Alloc Rec, U, was considered as a proxy for Kapton® (adhesive).

Table S2. Dataset for the production of 1 kg of battery cells: LFP. The source of information used is mentioned in the name

Dataset	Amount	Units
UF Output		
Li-ion battery cell production_LFP	Alloc Rec, U_RSE	1.00E+00	kg
Materials/Fuels Input		
Transport, freight train {GLO}| market group for	Alloc Rec, U	2.30E-01	tkm
Transport, freight, lorry 16-32 metric ton, EURO6 {GLO}| market for	Alloc Rec, U	5.10E-02	tkm
Positive electrode material for Li-ion battery_LFP	Alloc Rec, U_RSE	3.63E-01	kg
Negative carbonaceous electrode material for Li-ion battery_LFP	Alloc Rec, U_RSE	1.87E-01	kg
Electrode substrate for Li-ion battery_positive electrode| Alloc Rec, U_RSE	7.01E-02	kg
Electrode substrate for Li-ion battery_negative electrode	Alloc Rec, U_RSE	1.20E-01	kg
Electrolyte for Li-ion battery, 1M LiPF6 {GLO}| production	Alloc Rec, U_Ellingsen_2013_RSE	2.00E-01	kg
Battery separator production	Alloc Rec, U_Majeau-Bettez_2011_RSE	2.00E-02	kg
Li-ion battery production_Cell container sub-component: tab, aluminum	Alloc Rec, U_Ellingsen_2013_RSE	2.00E-03	kg
Li-ion battery production_Cell container sub-component: tab, copper	Alloc Rec, U_Ellingsen_2013_RSE	2.00E-03	kg
Li-ion battery production_Cell container sub-component: multilayer pouch	Alloc Rec, U_Ellingsen_2013_RSE	3.01E-02	kg
Polyol {RER}| production	Alloc Rec, U	5.00E-03	kg
Electricity/Heat		
Electricity, medium voltage {IT}| Electricity Production mix| Alloc Rec, U_RSE	2.38E+01	MJ

Table S3. Dataset for the production of 1 kg of battery cells: NMC 532 and NMC 622. The source of information used is mentioned in the name.

Dataset	Amount	Units
UF Output		
Li-ion battery cell production_NMC xyz	Alloc Rec, U_RSE	1.00E+00	kg
Materials/Fuels Input		
Transport, freight train {GLO}	market group for	Alloc Rec, U	2.30E-01	tkm
Transport, freight, lorry 16–32 metric ton, EURO6 {GLO}	market for	Alloc Rec, U	5.10E-02	tkm
NMC532: Positive electrode material for Li-ion battery_NMC532	Alloc Rec, U_RSE NMC622: Positive electrode material for Li-ion battery_NMC622	Alloc Rec, U_RSE	4.08E-01	kg
NMC 532: Negative carbonaceous electrode material for Li-ion battery_NMC532	Alloc Rec, U_RSE NMC622: Negative carbonaceous electrode material for Li-ion battery_NMC622	Alloc Rec, U_RSE	2.20E-01	kg
Electrode substrate for Li-ion battery_positive electrode| Alloc Rec, U_RSE	4.93E-02	kg
Electrode substrate for Li-ion battery_negative electrode	Alloc Rec, U_RSE	8.44E-2	kg
Electrolyte for Li-ion battery, 1M LiPF6 {GLO}	production	Alloc Rec, U_Ellingsen_2013_RSE	1.97E-1	kg
Battery separator production	Alloc Rec, U_Majeau-Bettez_2011_RSE	1.41E-02	kg

Dataset	Amount	Units
Li-ion battery production_Cell container sub-component: tab, aluminum Ι Alloc Rec, U_Ellingsen_2013_RSE	1.40E-03	kg
Li-ion battery production_Cell container sub-component: tab, copper Ι Alloc Rec, U_Ellingsen_2013_RSE	1.40E-03	kg
Li-ion battery production_Cell container sub-component: multilayer pouch Ι Alloc Rec, U_Ellingsen_2013_RSE	2.11E-02	kg
Polyol {RER}Ι production Ι Alloc Rec, U	3.50E-03	kg
Electricity/Heat		
Electricity, medium voltage {IT}Ι Electricity Production mixΙ Alloc Rec, U_RSE	3.76E+01	MJ

2.1.2.1 Electrodes: Anode and Cathode

Inside each cell, there are two electrodes: the positive electrode (cathode) and the negative electrode (anode). The positive electrode (cathode) is covered by electro-chemical active materials, an aggregate (binder), and a support (graphite). In this study, the active materials were lithium iron phosphate ($LiFePO_4$) for the LFP batteries and lithium–nickel–cobalt–manganese oxide ($LiNi_xCo_yMn_zO_2$) for the NMCs.

For NMC cells, the binder was polyvinylidene difluoride (PVDF), while the mixture of polyacrylate with carboxymethyl cellulose (CMC) was employed in LFP cells (Figure S3.). The used solvents were water for LFP and N-methyl-pyrrolidone (NMP) for NMCs. Solvents evaporated after the application of electrode pastes to current collectors.

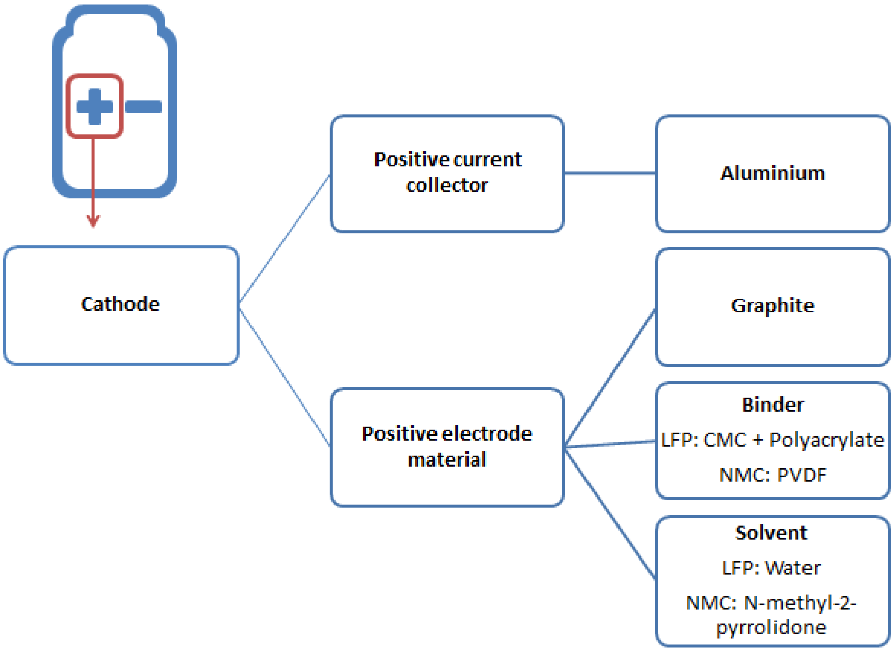

Figure S3. Composition diagram of the positive electrode for both LFP and NMC chemistry (CMC: carboxymethyl cellulose; PVDF: polyvinylidene difluoride)

For the LFP battery cells, lithium–iron–phosphate production was modelled according to Majeau-Bettez et al. [3], considering the following chemical reaction (Equation (1)) while assuming a 95% efficiency:

$$3\ LiOH_{(aq)} + H_3PO_{4(aq)} + FeSO_{4(aq)} \rightarrow LiFePO_{4(s)} + Li_2SO_{4(aq)} + 3H_2O \quad (1)$$

For NMCs, lithium–nickel–cobalt–manganese oxide was modelled in SimaPro, according to Majeau-Bettez et al. [3]. The authors did not include in the inventory H_2O and O_2 as input or H_2O emissions as output, but in the present study, these were considered (Table S5. Dataset for NMC 532 and Table S6. Dataset for NMC 622).

The equation relating to this reaction is the following (Equation (**Error! Reference source not found.**)):

$$Ni_xCo_yMn_z(OH)_2 + LiOH.H_2O + 0.25O_2 \rightarrow LiNi_xCo_yMn_zO_2 + 2.5H_2O \quad (2)$$

$Ni_xCo_yMn_z(OH)_2$ and $CoSO_4$ were modelled according to Majeau-Bettez et al. [3]. For $Ni_xCo_yMn_z(OH)_2$, the quantity of the different metals ($Ni_5Co_3Mn_2(OH)_2$ and $Ni_6Co_2Mn_2(OH)_2$) was adapted.

The following tables summarize the datasets related to the production of positive electrodes for the LFP (Table S4), NMC 532 (Table S5), and NMC 622 (Table S6) batteries.

Table S4. Dataset for the production of the positive electrode for LFP cells. The source of information used is mentioned in the name

Dataset	Amount	Units
UF Output		
Positive electrode material for Li-ion battery_LFP ǀ Alloc Rec, U_RSE	5.37E-01	kg
Materials/Fuels Input		
Transport, freight train {GLO}ǀ market group for ǀ Alloc Rec, U	2.04E+00	tkm
Transport, freight, lorry 16–32 metric ton, EURO6 {GLO}ǀ market for ǀ Alloc Rec, U	3.76E-01	tkm
Carboxymethyl cellulose, powder {GLO}ǀ market for ǀ Alloc Rec, U_RSE	8.90E-03	kg
Lithium iron phosphate {GLO}ǀ production ǀ Alloc Rec, U_Majeau-Bettez_2011_RSE	5.04E-01	kg
Carbon black {GLO}ǀ market for ǀ Alloc Rec, U RSE	1.19E-02	kg
Methyl acrylate {GLO}ǀ market for ǀ Alloc Rec, U_RSE	1.19E-02	kg
Water, deionized, from tap water, at user {Europe without Switzerland}ǀ market for water, deionized, from tap water, at user ǀ Alloc Rec, U	4.63E-01	kg
Emissions		
Water	4.63E-01	kg

Table S5. Dataset for the production of the positive electrode for NMC 532 cells. The source of information used is mentioned in the name

Dataset	Amount	Units
UF Output		
Positive electrode material for Li-ion battery_NMC 532 ǀ Alloc Rec, U_RSE	4.92E-01	kg
Materials/Fuels Input		
Transport, freight train {GLO}ǀ market group for ǀ Alloc Rec, U	1,87E+00	tkm
Transport, freight, lorry 16–32 metric ton, EURO6 {GLO}ǀ market for ǀ Alloc Rec, U	3,44E-01	tkm
Lithium nickel cobalt manganese oxide_532 {GLO}ǀ production ǀ Alloc Rec, U_Majeau-Bettez_2011_RSE	4,66E-01	kg
Carbon black {GLO}ǀ market for ǀ Alloc Rec, U RSE	1,70E-02	kg
N-methyl-2-pyrrolidone {GLO}ǀ market for ǀ Alloc Rec, U	5,08E-01	kg
Polyvinyl fluoride {GLO}ǀ market for ǀ Alloc Rec, U	8,48E-03	kg
Emissions		
1-methyl-2-pyrrolidinone	5.08E-01	kg

Table S6. Dataset for the production of the positive electrode for NMC 622 cells. The source of information used is mentioned in the name

Dataset	Amount	Units
UF Output		
Positive electrode material for Li-ion battery_NMC 622 ǀ Alloc Rec, U_RSE	4.64E-01	kg

Dataset	Amount	Units
Materials/Fuels Input		
Transport, freight train {GLO}∣ market group for ∣ Alloc Rec, U	1.76E+00	tkm
Transport, freight, lorry 16–32 metric ton, EURO6 {GLO}∣ market for ∣ Alloc Rec, U	3.25E-01	tkm
Lithium nickel cobalt manganese oxide_622 {GLO}∣ production ∣ Alloc Rec, U_Majeau-Bettez_2011_RSE	4.40E-01	kg
Carbon black {GLO}∣ market for ∣ Alloc Rec, U	1.60E-02	kg
N-methyl-2-pyrrolidone {GLO}∣ market for ∣ Alloc Rec, U	4.80E-01	kg
Polyvinyl fluoride {GLO}∣ market for ∣ Alloc Rec, U	8.00E-03	kg
Emissions		
1-methyl-2-pyrrolidinone	4.80E-01	kg

Datasets related to the production of lithium–iron–phosphate oxide for LFP batteries (Table S7) and lithium–nickel–cobalt–manganese oxide for NMC 532 (Table S8) and NMC 622 batteries (Table S9Table S9. Dataset) are summarized below.

Table S7. Dataset for the production of 1 kg of lithium–iron–phosphate oxide for LFP battery cells. The source of information used is mentioned in the name

Dataset	Amount	Units
UF Output		
Lithium iron phosphate {GLO}∣ production ∣ Alloc Rec, U_Majeau-Bettez_2011_RSE	1.00E+00	kg
Materials/Fuels Input		
Chemical factory, organics {GLO}∣ market for ∣ Alloc Rec, U	4.00E-10	p
Lithium hydroxide {GLO}∣ market for ∣ Alloc Rec, U_RSE	4.60E-01	kg
Transport, freight train {GLO}∣ market group for ∣ Alloc Rec, U	1.30E+00	tkm
Transport, freight, lorry 16–32 metric ton, EURO6 {GLO}∣ market for ∣ Alloc Rec, U	2.10E-01	tkm
Phosphoric acid, industrial grade, without water, in 85% solution state {GLO}∣ market for ∣ Alloc Rec, U	6.50E-01	kg
Iron sulfate {GLO}∣ market for ∣ Alloc Rec, U	1.00E+00	kg
Water, deionized, from tap water, at user {GLO}∣ market for ∣ Alloc Rec, U	4.60E+01	kg
Electricity/Heat		
Heat, district or industrial, natural gas {RoW}∣ market for heat, district or industrial, natural gas ∣ Alloc Rec, U	1.50E+01	MJ
Emissions		
Heat and waste	1.50E+00	MJ
Lithium	9.26E-02	kg
Iron	1.90E-02	kg
Phosphate	3.30E-02	kg
Sulfate	6.41E-01	kg

Table S8. Dataset for the production of 1 kg of lithium–nickel–cobalt–manganese oxide for NMC 532 battery cells. The source of information used is mentioned in the name

Dataset	Amount	Units
UF Output		
Lithium nickel cobalt manganese oxide_532 {GLO}∣ production ∣ Alloc Rec, U_Majeau-Bettez_2011_RSE	1.00E+00	kg
Materials/Fuels Input		
Chemical factory, organics {GLO}∣ market for ∣ Alloc Rec, U	4.60E-10	p

Dataset	Amount	Units
Lithium hydroxide {GLO}| market for | Alloc Rec, U	2.50E-01	kg
Transport, freight train {GLO}| market group for | Alloc Rec, U	7.20E-01	tkm
Transport, freight, lorry 16–32 metric ton, EURO6 {GLO}| market for | Alloc Rec, U	1.20E-01	tkm
Ni0.5Co0.2Mn0.3(OH)2 | Alloc Rec, U_RSE	9.50E-01	kg
Water, deionized, from tap water, at user {Europe without Switzerland}| market for water, deionized, from tap water, at user | Alloc Rec, U	1.86E-01	kg
Oxygen, liquid {RER}| market for | Alloc Rec, U	8.29E-02	kg
Electricity/Heat		
Heat, district or industrial, natural gas {Europe without Switzerland}| market for heat, district or industrial, natural gas | Alloc Rec, U	5.50E-01	MJ
Emissions		
Heat and waste	5.50E+00	MJ
Water	4.66E-01	kg

Table S9. Dataset for the production of 1 kg of lithium–nickel–cobalt–manganese oxide for NMC 622 battery cells. The source of information used is mentioned in the name

Dataset	Amount	Units
UF Output		
Lithium nickel cobalt manganese oxide_622 {GLO}| production | Alloc Rec, U_Majeau-Bettez_2011_RSE	1.00E+00	kg
Materials/Fuels Input		
Chemical factory, organics {GLO}| market for | Alloc Rec, U	4.60E-10	P
Lithium hydroxide {GLO}| market for | Alloc Rec, U	2.50E-01	kg
Transport, freight train {GLO}| market group for | Alloc Rec, U	7.20E-01	tkm
Transport, freight, lorry 16–32 metric ton, EURO6 {GLO}| market for | Alloc Rec, U	1.20E-01	tkm
Ni0.6Co0.2Mn0.2(OH)2 | Alloc Rec, U_RSE	9.50E-01	kg
Water, deionized, from tap water, at user {Europe without Switzerland}| market for water, deionized, from tap water, at user | Alloc Rec, U	1.86E-01	kg
Oxygen, liquid {RER}| market for | Alloc Rec, U	8.25E-02	kg
Electricity/Heat		
Heat, district or industrial, natural gas {Europe without Switzerland}| market for heat, district or industrial natural gas | Alloc Rec, U	5.50E-01	MJ
Emissions		
Heat and waste	5.50E+00	MJ
Water	4.64E-01	kg

The negative electrode (anode) consists of the following materials (Figure S4.).

- Graphite.
- Binder.
    - Carboxymethyl cellulose (CMC) and styrene–butadiene rubber (SBR) for LFP cells.
        - CMC and poly acrylic acid (PAA) for NMC cells.
- Solvent (water or N-methyl pyrrolidone), which evaporates after application to the substrate.

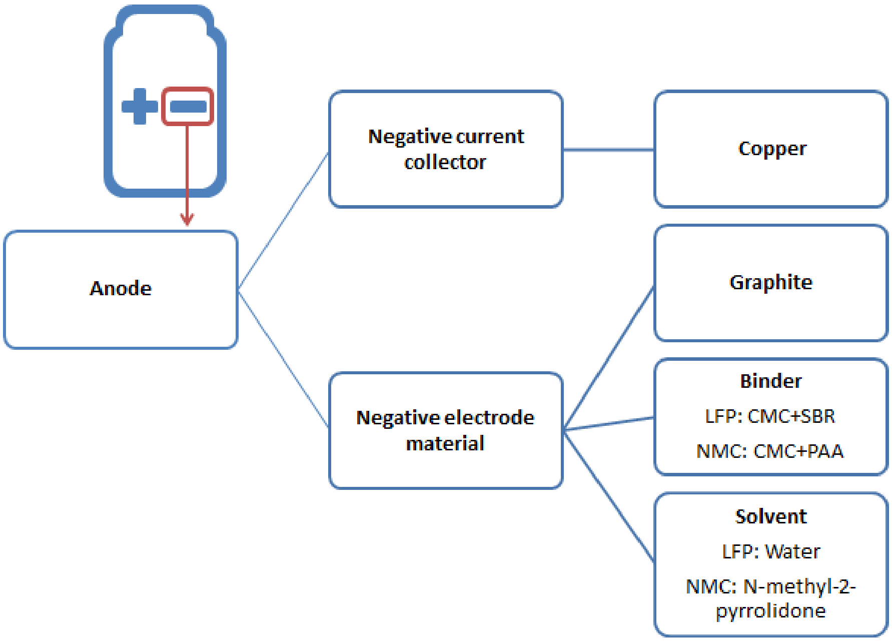

Figure S4. Composition diagram of the negative electrode for both LFP and NMC chemistries (CMC: carboxymethyl cellulose; SBR: styrene–butadiene rubber; PAA: poly acrylic acid).

The following tables summarize the datasets related to the production of negative electrodes for the LFP (Table S10), NMC 532, and NMC 622 (Table S11) batteries.

Table S10. Dataset for the production of 1 kg of negative electrode for LFP cells. The source of information used is mentioned in the name

Dataset	Amount	Units
UF Output		
Negative carbonaceous electrode material for Li-ion battery_LFP ǀ Alloc Rec, U_RSE	5.01E-01	kg
Materials/Fuels Input		
Graphite, battery grade {RoW}ǀ production ǀ Alloc Rec, U	4.83E-01	kg
Transport, freight train {GLO}ǀ market group for ǀ Alloc Rec, U	1.00E-01	tkm
Transport, freight, lorry 16–32 metric ton, EURO6 {GLO}ǀ market for ǀ Alloc Rec, U	5.01E-02	tkm
Carboxymethyl cellulose, powder {GLO}ǀ market for ǀ Alloc Rec, U_RSE	8.04E-03	kg
Acrylonitrile–butadiene–styrene copolymer {RER}ǀ production ǀ Alloc Rec, U	1.07E-02	kg
Water, deionized, from tap water, at user {RoW}ǀ market for water, deionized, from tap water, at user ǀ Alloc Rec, U	4.99E-01	kg
Emissions		
Water	4.99E-01	kg

Table S11. Dataset for the production of 1 kg of negative electrode for NMC 532 and NMC 622 cells. The source of information used is mentioned in the name

Dataset	Amount	Units
UF Output		
Negative carbonaceous electrode material for Li-ion battery_NMC ǀ Alloc Rec, U_RSE	5.02E-01	kg
Materials/Fuels Input		
Graphite, battery grade {RoW}ǀ production ǀ Alloc Rec, U	4.83E-01	kg
Transport, freight train {GLO}ǀ market group for ǀ Alloc Rec, U	1.00E-01	tkm
Transport, freight, lorry 16–32 metric ton, EURO6 {GLO}ǀ market for ǀ Alloc Rec, U	5.02E-02	tkm

Dataset	Amount	Units
Carboxymethyl cellulose, powder {GLO}∣ market for ∣ Alloc Rec, U_RSE	9.66E-03	kg
Acrylonitrile–butadiene–styrene copolymer {RER}∣ production ∣ Alloc Rec, U	9.66E-03	kg
Water, deionized, from tap water, at user {Europe without Switzerland}∣ market for water, deionized, from tap water, at user ∣ Alloc Rec, U	4.98E-01	kg
Emissions		
Water	4.98E-01	kg

The electrode's metal surface layer measures approximately 15–20 μm. This layer requires adequate support to perform its function as a current collector; aluminum was used as substrate for the positive electrode, while copper was used for the negative one. Data and information contained within the datasets related to the substrate for the positive electrode (Table S12) and the substrate for the negative electrode (Table S13) are reported in the following tables.

For the dataset relating to the production of the copper substrate, it was possible to carry out a regionalization starting from the already available dataset in Ecoinvent Copper {GLO} ∣ market for ∣ Alloc Rec, U at the European level, taking the European production data for 2016 (as provided by the European Copper Institute) into account [4].

Table S12. Dataset for the production of 1 kg of electrode substrate for positive electrode for both LFP and NMC cells. The source of information used is mentioned in the name

Dataset	Amount	Units
UF Output		
Electrode substrate for Li-ion battery, positive electrode∣ Alloc Rec, U_RSE	1.00E+00	kg
Materials/Fuels Input		
Transport, freight train {GLO}∣ market group for ∣ Alloc Rec, U	2.00E-01	tkm
Transport, freight, lorry 16–32 metric ton, EURO6 {GLO}∣ market for ∣ Alloc Rec, U	1.00E-01	tkm
Metal working factory {GLO}∣ market for ∣ Alloc Rec, U	4.00E-10	p
Aluminum, primary, ingot {IAI Area 2, without Quebec}∣ production ∣ Alloc Rec, U	1.00E+00	kg
Sheet rolling, aluminum {GLO}∣ market for ∣ Alloc Rec, U_RSE	1.00E+00	kg
Electricity/Heat		
Electricity, high voltage {UCTE}∣ production mix ∣ Alloc Rec, U	4.6E-10	MJ

Table S13. Dataset for the production of 1 kg of electrode substrate for negative electrode for both LFP and NMC cells. The source of information used is mentioned in the name

Dataset	Amount	Units
UF Output		
Electrode substrate for Li-ion battery_negative electrode ∣ Alloc Rec, U_RSE	1.00E+00	kg
Materials/Fuels Input		
Transport, freight train {GLO}∣ market group for ∣ Alloc Rec, U	2.00E-01	tkm
Transport, freight, lorry 16–32 metric ton, EURO6 {GLO}∣ market for ∣ Alloc Rec, U	1.00E-01	tkm
Metal working factory {RER}∣ construction ∣ Alloc Rec, U	4.00E-10	p
Copper {RER}∣ market for ∣ Alloc Rec, U_RSE	1.00E+00	kg
Sheet rolling, copper {RER}∣ processing ∣ Alloc Rec, U	1.00E+00	kg
Electricity/Heat		
Electricity, high voltage {UCTE}∣ production mix ∣ Alloc Rec, U	4.6E-10	MJ

2.1.2.2 Separator

The separator's role is to prevent electrodes (anode and cathode) from touching while electrons flow in the electrolyte with as little resistance as possible. In this study, the same separator was used both for LFP and NMC batteries. The inventory for the production of the separator was assumed to follow the study of Majeau-Bettez et al. [3], where it was presumed to be composed of polypropylene (PP) and polyethylene (PE) in equal amounts.

2.1.2.3 Electrolyte

The electrolyte was made of lithium salt ($LiPF_6$) and solvents. In this study, the inventory for the production of electrolyte was assumed to follow the work of Ellingsen et al. [1]

2.1.2.4 Multilayer pouch

The cell container consisted of a multilayer pouch that surrounded the other battery cell components and two tabs. In this study, the inventory to produce tabs and multilayer pouches was assumed to follow the work of Ellingsen et al. [1].

2.1.3 Battery Packaging

Packaging is divided into three sub-components: module packaging, battery retention, and battery tray. In this study, the inventory for the production of tabs and multilayer pouches was assumed to follow the work of Ellingsen et al. [1]

2.1.4 Battery Management System (BMS)

The battery management system (BMS) includes battery module boards, an integrated battery interface system (IBIS), fasteners, a high voltage (HV) system, and a low voltage system. In this study, the inventory for the production of the BMS was assumed to follow the work of Ellingsen et al. [1].

2.1.5 Cooling Circuit

For thermal management, a battery is equipped with a cooling circuit. In this study, the inventory for the production of a cooling circuit was assumed to follow the work of Ellingsen et al. [1].

2.2 Use Phase

The use phase consists of charging and discharging the battery.

The Italian manufacturer of stationary systems that provided the primary data estimates that, during the entire useful life and for both LFP and NMC batteries, the storage devices can perform up to ≈5000 charge-discharge cycles while maintaining their efficiency. This condition happens if batteries work under "ideal" (no stress) conditions: operating temperatures between 5 and 30 °C, avoiding complete discharge and maintaining an average charge of around 50%.

Two different scenarios were considered to model the batteries' use phases:

Scenario A: generic-use (Table S14)

A generic use scenario. The considered energy mix was the Italian one, updated to 2018, as defined in [2].

Scenario B: INECP (Integrated National Energy and Climate Plan) scenario [5]—control of over production from non-programmable renewable plants below 1 TWh in 2030 (Table S15).

In this scenario, batteries were used to provide services to the grid in accordance with the objectives of the Italian INECP [5] in order to limit over production from non-programmable renewable sources (wind and solar) to plants below 1 TWh, according to the estimates of use illustrated in [6]. In this scenario, batteries were recharged with the energy produced by photovoltaic and wind power, and, in the discharge phase, they avoided the production of energy from fossil sources—from natural gas plants in a combined cycle, in particular. As shown in Figure S5. , no full charges and discharges were expected, and, therefore, the battery life was not limited by the number of cycles suggested by the manufacturer (5000). Battery life was estimated to be limited to 10 years. For this scenario, the quantity of battery capacity that was used for each kWh released by the batteries was 1.20E-03 kWh. The considered storage systems were capable of storing approximately 83.3 kWh/year for each kWh of installed capacity.

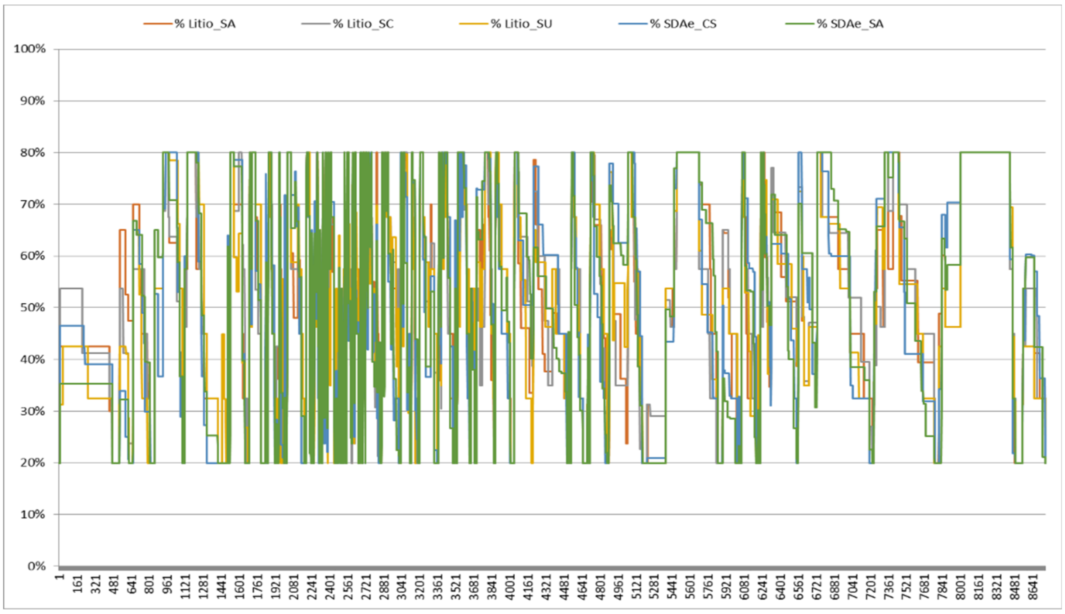

Figure S5. Operation hypothesized in [6] relating to a typical year according to the NECP hypotheses. The initials in the legend downstream of the lithium wording indicate the market area

Table S14. Dataset for the use phase; Scenario A (XXX represents the type of battery: LFP, NMC 532, or NMC 622)

Dataset	Amount	Units
UF Output		
Scenario A_Use_XXX RSE ǀ Alloc Rec, U_RSE	1.00E+00	kWh
Materials/Fuels Input		
Li-ion battery production_1 Battery pack_1kWhǀ Alloc Rec, U_XXX_RSE	2.00E-04	kWh
Electricity/Heat		
Electricity, medium voltage {IT}ǀ Electricity Production mixǀ Alloc Rec, U_RSE	1.00E-01	kWh
Emissions		
Heat and waste	1.00E-01	kWh

Table S15. Dataset for the use phase; Scenario B (XXX represents the type of battery: LFP, NMC 532, or NMC 622)

Dataset	Amount	Units
UF Output		
Scenario B_Use_XXX RSE ǀ Alloc Rec, U_RSE	1.00E+00	kWh
Avoided Products		
Electricity, high voltage {IT}ǀ electricity production, natural gas, in CC PNIEC ǀ Alloc Rec, U—RSE	1.00E+00	kWh
Materials/Fuels Input		
Li-ion battery production_1 Battery pack_1kWhǀ Alloc Rec, U_XXX_RSE	1.20E-03	kWh
Electricity/Heat		
FRNP_Electricity, high voltage {IT}ǀ Electricity mix 2030 PNIEC ǀ Alloc Rec, U_RSE_v2020	1.10E+00	kWh

Dataset	Amount	Units
Emissions		
Heat and waste	1.00E-01	kWh

2.3 End-of-Life

The end-of-life modelling was carried out starting from the information reported by Mohr et al. [7] and the datasets present in Ecoinvent related to the pyrometallurgical treatment (used Ni-metal hydride battery (GLO) | treatment of used Ni-metal hydride battery, pyrometallurgical treatment) and the hydrometallurgical treatment (used Li-ion battery (GLO) | treatment of used Li-ion battery, hydrometallurgical treatment) of exhausted batteries.

It was assumed that batteries were subjected to 50% of pyrometallurgical treatment and 50% of the hydrometallurgical one.

When applied to the LFP battery, the pyrometallurgical process allows for the recovery of aluminum and copper from the cells. When the pyrometallurgical process is applied to the NMC 532 and NMC 622 batteries, it also allows for the recovery of cobalt, nickel, and manganese salts.

The hydrometallurgical process allows for the recovery of aluminum, copper, and lithium salts for all considered batteries, and the recycling of cobalt, nickel, and manganese salts only for the NMCs.

In this study, as reported by Mohr et al. [7], the recovery rate of metals and salts was equal to 93.6%. Table S16 summarizes what was previously described, highlighting recovered metals and salts thanks to the pyrometallurgical and hydrometallurgical processes.

Table S16. Metals and salts recovered during the end-of-life processes for the analyzed batteries. EoL: end-of-life

Chemistry	EoL treatment	Recovered materials					
		Al	Cu	Co salts	Ni salts	Mn salts	Li salts
LFP	Pyrometallurgical	X	X				
	Hydrometallurgical	X	X				X
NMC 532	Pyrometallurgical	X	X	X	X	X	
	Hydrometallurgical	X	X	X	X	X	X
NMC 622	Pyrometallurgical	X	X	X	X	X	
	Hydrometallurgical	X	X	X	X	X	X

Regarding other battery components, the following datasets present within Ecoinvent were identified.

- Packaging: a treatment and recycling process of mixed plastics was considered (mixed plastics (waste treatment) (GLO) | recycling of mixed plastics).
- BMS and cooling system: a mechanical treatment of electronic waste was considered (used industrial electronic device (GLO) | treatment of, mechanical treatment).

The following tables show all datasets considered to model the end-of-life phase of the LFP (Table S17), NMC 532 (Table S18), and NMC 622 (Table S19) batteries.

Table S17. Dataset for the use phase of 1 kg of LFP batteries. The source of information used is mentioned in the name

Dataset	Amount	Units
Waste specification		
LFP RSE EoL_1 kg | Alloc Rec, U_RSE	1.00E+00	kg
Outputs to Technosphere: Waste and Emissions to Treatment		
LFP RSE_pyrometallurgical treatment | Alloc Rec, U_RSE	6.00E-01 * 0.5	kg
LFP RSE_hydrometallurgical treatment | Alloc Rec, U_RSE	6.00E-01 * 0.5	kg
Mixed plastics (waste treatment) {GLO}| recycling of mixed plastics | Alloc Rec, U	3.20E-01	kg

Dataset	Amount	Units
Used industrial electronic device {GLO}| treatment of, mechanical treatment | Alloc Rec, U	3.70E-02	kg
Used industrial electronic device {GLO}| treatment of, mechanical treatment | Alloc Rec, U	4.10E-02	kg

Table S18. Dataset for the use phase of 1 kg of NMC 532 batteries. The source of information used is mentioned in the name

Dataset	Amount	Units
Waste specification		
NMC 532 RSE EoL_1 kg | Alloc Rec, U_RSE	1.00E+00	kg
Outputs to Technosphere: Waste and Emissions to Treatment		
NMC532 RSE_pyrometallurgical treatment | Alloc Rec, U_RSE	6.00E-01 * 0.5	kg
NMC532 RSE_ hydrometallurgical treatment | Alloc Rec, U_RSE	6.00E-01 * 0.5	kg
Mixed plastics (waste treatment) {GLO}| recycling of mixed plastics | Alloc Rec, U	3.20E-01	kg
Used industrial electronic device {GLO}| treatment of, mechanical treatment | Alloc Rec, U	3.70E-02	kg
Used industrial electronic device {GLO}| treatment of, mechanical treatment | Alloc Rec, U	4.10E-02	kg

Table S19. Dataset for the use phase of 1 kg of NMC 622 batteries. The source of information used is mentioned in the name

Dataset	Amounts	Units
Waste specification		
NMC 622 RSE EoL_1 kg | Alloc Rec, U_RSE	1,00E+00	kg
Outputs to Technosphere: Waste and Emissions to Treatment		
NMC622 RSE_pyrometallurgical treatment | Alloc Rec, U_RSE	6.00E-01 * 0.5	kg
NMC622 RSE_ hydrometallurgical treatment | Alloc Rec, U_RSE	6.00E-01 * 0.5	kg
Mixed plastics (waste treatment) {GLO}| recycling of mixed plastics | Alloc Rec, U	3.20E-01	kg
Used industrial electronic device {GLO}| treatment of, mechanical treatment | Alloc Rec, U	3.70E-02	kg
Used industrial electronic device {GLO}| treatment of, mechanical treatment | Alloc Rec, U	4.10E-02	kg

The following tables (Table S20–25) summarize the information contained within the datasets related to hydrometallurgical and pyrometallurgical processes for the LFP, NMC 532, and NMC 622 battery cells.

Table S20. Dataset related to the hydrometallurgical process for 1 kg of LFP cell. The source of information used is mentioned in the name. The negative sign inputs correspond to avoided products thanks to end-of-life treatments

Dataset	Amount	Units
UF Output		
LFP RSE_hydrometallurgical treatment | Alloc Rec, U_RSE	1.00E+00	kg
Avoided Products		
Water of unspecified natural origin and GLO	7.20E-01	l
Materials/Fuels Input		
Lime, hydrated, packed {GLO}| market for | Alloc Rec, U	1.16E-01	kg
Chemical factory, organics {GLO}| market for | Alloc Rec, U	4.00E-10	p
Sulfuric acid {GLO}| market for | Alloc Rec, U	2.13E-01	kg
Chemical, inorganic {GLO}| market for chemicals, inorganic | Alloc Rec, U	2.50E-02	kg
Lithium hydroxide {GLO}| market for | Alloc Rec, U	−1.63E-01	kg

Dataset	Amount	Units
Electrolyte for Li-ion battery, 1M LiPF6 {GLO}∣ production ∣ Alloc Rec, U_Majeau-Bettez_RSE	−2.25E-03	kg
Aluminum, primary, ingot {IAI Area 2, without Quebec}∣ production ∣ Alloc Rec, U	−6.56E-02	kg
Copper {RER}∣ market for ∣ Alloc Rec, U_RSE	−1.13E-01	kg
Aluminum alloy, metal matrix composite {GLO}∣ market for ∣ Alloc Rec, U	−1.87E-03	kg
Copper {RER}∣ production, primary ∣ Alloc Rec, U	−1.59E-03	kg
Copper {GLO}∣ market for ∣ Alloc Rec, U	−2.81E-04	kg
Aluminum alloy, metal matrix composite {GLO}∣ market for ∣ Alloc Rec, U	−1.41E-02	kg
Electricity/Heat		
Electricity, medium voltage {IT}∣ Electricity Production mix∣ Alloc Rec, U_RSE	1.40E-01	kWh
Emissions—Air		
Sulfur dioxide	4.50E-06	kg
NMVOC (non-methane volatile organic compound) of unspecified origin	2.50E-06	kg
Emissions—Water		
Unspecified hydrocarbons	1.00E-08	kg
Cobalt	1.67E-05	kg
COD (chemical oxygen demand)	3.00E-05	kg
Nickel	1.67E-05	kg
Fluoride	3.00E-08	kg
Copper	1.67E-05	kg
Unspecified suspended solids	1.20E-05	kg
Waste water/m3	3.37E-01	l
Waste Treatment		
Waste plastic, mixture {Europe without Switzerland}∣ treatment of waste plastic, mixture, municipal incineration ∣ Alloc Rec, U	9.95E-03	kg
Waste plastic, mixture {Europe without Switzerland}∣ treatment of waste plastic, mixture, sanitary landfill ∣ Alloc Rec, U	8.42E-03	kg
Waste plastic, mixture {Europe without Switzerland}∣ clinker production ∣ Alloc Rec, U	1.68E-02	kg

Table S21. Dataset related to the pyrometallurgical process for 1 kg of LFP cell. The source of information used is mentioned in the name. The negative sign inputs correspond to avoided products thanks to end-of-life treatments

Dataset	Amount	Units
UF Output		
LFP RSE_pyrometallurgical treatment ∣ Alloc Rec, U_RSE	1.00E+00	kg
Avoided Products		
Water of unspecified natural origin and GLO	1.00E-03	m3
Materials/Fuels Input		
Sodium hydroxide, without water, in 50% solution state {GLO}∣ market for ∣ Alloc Rec, U	2.10E-01	kg
Blister-copper conversion facility {GLO}∣ market for ∣ Alloc Rec, U	5.00E-10	p
Aluminum, primary, ingot {IAI Area 2, without Quebec}∣ production ∣ Alloc Rec, U	−6.56E-02	kg
Copper {RER}∣ market for ∣ Alloc Rec, U_RSE	−1.13E-01	kg
Aluminum alloy, metal matrix composite {GLO}∣ market for ∣ Alloc Rec, U	−1.87E-03	kg
Copper {RER}∣ production, primary ∣ Alloc Rec, U	−1.59E-03	kg
Copper {GLO}∣ market for ∣ Alloc Rec, U	−2.81E-04	kg
Aluminum alloy, metal matrix composite {GLO}∣ market for ∣ Alloc Rec, U	−1.41E-02	kg
Electricity/Heat		
Electricity, medium voltage {IT}∣ Electricity Production mix∣ Alloc Rec, U_RSE	8.00E-01	kWh

Dataset	Amount	Units
Emissions—Air		
Water/m3	0.00E+00	m3
Sulfur dioxide	4.80E-05	kg
Particulates, < 2.5 um	1.00E-04	kg
Particulates, > 10 um	1.04E-05	kg
Particulates, > 2.5 um and < 10 um	9.36E-05	kg
Emissions—Water		
Water and GLO	0.00E+00	l
Sulfate	0.00E+00	kg
Chloride	4.00E-02	kg
Sulfur dioxide	4.00E-02	kg
Waste water	1.00E+00	kg
Waste Treatment		
Waste plastic, mixture {Europe without Switzerland}| treatment of waste plastic, mixture, municipal incineration | Alloc Rec, U	9.95E-03	kg
Waste plastic, mixture {Europe without Switzerland}| treatment of waste plastic, mixture, sanitary landfill | Alloc Rec, U	8.42E-03	kg
Waste plastic, mixture {Europe without Switzerland}| clinker production | Alloc Rec, U	1.68E-02	kg

Table S22. Dataset related to the hydrometallurgical process for 1 kg of NMC 532 cell. The source of information used is mentioned in the name. The negative sign inputs correspond to avoided products thanks to end-of-life treatments

Dataset	Amount	Units
UF Output		
NMC532 RSE_ hydrometallurgical treatment | Alloc Rec, U_RSE	1.00E+00	kg
Avoided Products		
Water of unspecified natural origin and GLO	7.20E-01	l
Materials/Fuels Input		
Lime, hydrated, packed {GLO}| market for | Alloc Rec, U	1.16E-01	kg
Chemical factory, organics {GLO}| market for | Alloc Rec, U	4.00E-10	p
Sulfuric acid {GLO}| market for | Alloc Rec, U	2.13E-01	kg
Chemical, inorganic {GLO}| market for chemicals, inorganic | Alloc Rec, U	2.50E-02	kg
Lithium hydroxide {GLO}| market for | Alloc Rec, U	-8.60E-02	kg
Lithium hexafluorophosphate {GLO}| market for | Alloc Rec, U	−2.21E-03	kg
CoSO4 {GLO}| production | Alloc Rec, U_Majeau-Bettez_RSE	−1.16E-01	kg
NiSO4 {GLO} | Alloc Rec, U__Majeau-Bettez_RSE	−2.90E-01	kg
Manganese sulfate {GLO}| production | Alloc Rec, U_Majeau-Bettez_RSE	−1.70E-01	kg
Aluminum, primary, ingot {IAI Area 2, without Quebec}| production | Alloc Rec, U	−4.61E-02	kg
Copper {RER}| market for | Alloc Rec, U_RSE	−7.90E-02	kg
Aluminum alloy, metal matrix composite {GLO}| market for | Alloc Rec, U	−1.31E-03	kg
Copper {RER}| production, primary | Alloc Rec, U	−1.11E-03	kg
Copper {GLO}| market for | Alloc Rec, U	−1.97E-04	kg
Aluminum alloy, metal matrix composite {GLO}| market for | Alloc Rec, U	−9.87E-03	kg
Electricity/Heat		
Electricity, medium voltage {IT}| Electricity Production mix| Alloc Rec, U_RSE	1.40E-01	kWh
Emissions—Air		
Sulfur dioxide	4.50E-06	kg

Dataset	Amount	Units
Emissions—Water		
Water and GLO	3.37E-01	l
Unspecified hydrocarbons	1.00E-08	kg
Cobalt	1.67E-05	kg
Nickel	1.67E-05	kg
Fluoride	3.00E-08	kg
Copper	1.67E-05	kg
Unspecified suspended solids	1.20E-05	kg
Waste Treatment		
Waste plastic, mixture {Europe without Switzerland}∣ treatment of waste plastic, mixture, municipal incineration ∣ Alloc Rec, U	6.99E-03	kg
Waste plastic, mixture {Europe without Switzerland}∣ treatment of waste plastic, mixture, sanitary landfill ∣ Alloc Rec, U	8.42E-03	kg
Waste plastic, mixture {Europe without Switzerland}∣ clinker production ∣ Alloc Rec, U	1.18E-02	kg

Table S23. Dataset related to the pyrometallurgical process for 1 kg of NMC 532 cell. The source of information used is mentioned in the name. The negative sign inputs correspond to avoided products thanks to end-of-life treatments

Dataset	Amount	Units
UF Output		
NMC532 RSE_pyrometallurgical treatment ∣ Alloc Rec, U_RSE	1.00E+00	kg
Avoided Products		
Water of unspecified natural origin and GLO	1.00E+00	l
Materials/Fuels Input		
Blister-copper conversion facility {GLO}∣ market for ∣ Alloc Rec, U	5.00E-10	p
Sodium hydroxide, without water, in 50% solution state {GLO}∣ market for ∣ Alloc Rec, U	2.10E-01	kg
CoSO4 {GLO}∣ production ∣ Alloc Rec, U_Majeau-Bettez_RSE	−1.16E-01	kg
NiSO4 {GLO} ∣ Alloc Rec, U__Majeau-Bettez_RSE	−2.90E-01	kg
Manganese sulfate {GLO}∣ production ∣ Alloc Rec, U_Majeau-Bettez_RSE	−1.70E-01	kg
Aluminum, primary, ingot {IAI Area 2, without Quebec}∣ production ∣ Alloc Rec, U	−4.61E-02	kg
Copper {RER}∣ market for ∣ Alloc Rec, U_RSE	−7.90E-02	kg
Aluminum alloy, metal matrix composite {GLO}∣ market for ∣ Alloc Rec, U	−1.31E-03	kg
Copper {RER}∣ production, primary ∣ Alloc Rec, U	−1.11E-03	kg
Copper {GLO}∣ market for ∣ Alloc Rec, U	−1.97E-04	kg
Aluminum alloy, metal matrix composite {GLO}∣ market for ∣ Alloc Rec, U	−9.87E-03	kg
Electricity/Heat		
Electricity, medium voltage {IT}∣ Electricity Production mix∣ Alloc Rec, U_RSE	8.00E-01	kWh
Emissions—Air		
Sulfur dioxide	4.80E-05	kg
Particulates, < 2.5 um	1.00E-04	kg
Particulates, > 10 um	1.04E-05	kg
Particulates, > 2.5 um, and < 10um	9.36E-05	kg
Emissions—Water		
Waste water	1.00E+00	kg
Sulfur dioxide	4.00E-02	kg
Chloride	4.00E-02	kg
Waste Treatment		

Dataset	Amount	Units
Waste plastic, mixture {Europe without Switzerland}∣ treatment of waste plastic, mixture, municipal incineration ∣ Alloc Rec, U	6.99E-03	kg
Waste plastic, mixture {Europe without Switzerland}∣ treatment of waste plastic, mixture, sanitary landfill ∣ Alloc Rec, U	5.92E-03	kg
Waste plastic, mixture {Europe without Switzerland}∣ clinker production ∣ Alloc Rec, U	1.18E-02	kg

Table S24. Dataset related to the hydrometallurgical process for 1 kg of NMC 622 cell. The source of information used is mentioned in the name. The negative sign inputs correspond to avoided products thanks to end-of-life treatments

Dataset	Amount	Units
UF Output		
NMC622 RSE_hydrometallurgical treatment ∣ Alloc Rec, U_RSE	1.00E+00	kg
Avoided Products		
Water of unspecified natural origin and GLO	7.20E-01	l
Materials/Fuels Input		
Lime, hydrated, packed {GLO}∣ market for ∣ Alloc Rec, U	1.16E-01	kg
Chemical factory, organics {GLO}∣ market for ∣ Alloc Rec, U	4.00E-10	p
Sulfuric acid {GLO}∣ market for ∣ Alloc Rec, U	2.13E-01	kg
Chemical, inorganic {GLO}∣ market for chemicals, inorganic ∣ Alloc Rec, U	2.50E-02	kg
Lithium hydroxide {GLO}∣ market for ∣ Alloc Rec, U	−8.57E-02	kg
Lithium hexafluorophosphate {GLO}∣ market for ∣ Alloc Rec, U	−2.21E-03	kg
CoSO4 {GLO}∣ production ∣ Alloc Rec, U_Majeau-Bettez_RSE	−1.16E-01	kg
NiSO4 {GLO} ∣ Alloc Rec, U__Majeau-Bettez_RSE	−3.47E-01	kg
Manganese sulfate {GLO}∣ production ∣ Alloc Rec, U_Majeau-Bettez_RSE	−1.13E-01	kg
Aluminum, primary, ingot {IAI Area 2, without Quebec}∣ production ∣ Alloc Rec, U	−4.61E-02	kg
Copper {RER}∣ market for ∣ Alloc Rec, U_RSE	−7.90E-02	kg
Aluminum alloy, metal matrix composite {GLO}∣ market for ∣ Alloc Rec, U	−1.31E-03	kg
Copper {RER}∣ production, primary ∣ Alloc Rec, U	−1.11E-03	kg
Copper {GLO}∣ market for ∣ Alloc Rec, U	−1.97E-04	kg
Aluminum alloy, metal matrix composite {GLO}∣ market for ∣ Alloc Rec, U	−9.87E-03	kg
Electricity/Heat		
Electricity, medium voltage {IT}∣ Electricity Production mix∣ Alloc Rec, U_RSE	1.40E-01	kWh
Emissions—Air		
Sulfur dioxide	4.50E-06	kg
NMVOC (non-methane volatile organic compound) of unspecified origin	2.50E-06	kg
Emissions—Water		
Water and GLO	3.37E-01	l
Unspecified hydrocarbons	1.00E-08	kg
Cobalt	1.67E-05	kg
COD (chemical oxygen demand)	3.00E-05	kg
Nickel	1.67E-05	kg
Fluoride	3.00E-08	kg
Copper	1.67E-05	kg
Unspecified suspended solids	1.20E-05	kg
Waste Treatment		
Waste plastic, mixture {Europe without Switzerland}∣ treatment of waste plastic, mixture, municipal incineration ∣ Alloc Rec, U	6.99E-03	kg

Dataset	Amount	Units
Waste plastic, mixture {Europe without Switzerland}ǀ treatment of waste plastic, mixture, sanitary landfill ǀ Alloc Rec, U	5.92E-03	kg
Waste plastic, mixture {Europe without Switzerland}ǀ clinker production ǀ Alloc Rec, U	1.18E-02	kg

Table S25. Dataset related to the pyrometallurgical process for 1 kg of NMC 622 cell. The source of information used is mentioned in the name. The negative sign inputs correspond to avoided products thanks to end-of-life treatments

Dataset	Amount	Units
UF Output		
NMC622 RSE_pyrometallurgical treatment ǀ Alloc Rec, U_RSE	1.00E+00	kg
Avoided Products		
Water of unspecified natural origin and GLO	1.00E+00	l
Materials/Fuels		
Blister-copper conversion facility {GLO}ǀ market for ǀ Alloc Rec, U	5.00E-10	p
Sodium hydroxide, without water, in 50% solution state {GLO}ǀ market for ǀ Alloc Rec, U	2.10E-01	kg
CoSO4 {GLO}ǀ production ǀ Alloc Rec, U_Majeau-Bettez_RSE	−1.16E-01	kg
NiSO4 {GLO} ǀ Alloc Rec, U__Majeau-Bettez_RSE	−3.47E-01	kg
Manganese sulfate {GLO}ǀ production ǀ Alloc Rec, U_Majeau-Bettez_RSE	−1.13E-01	kg
Aluminum, primary, ingot {IAI Area 2, without Quebec}ǀ production ǀ Alloc Rec, U	−4.61E-02	kg
Copper {RER}ǀ market for ǀ Alloc Rec, U_RSE	−7.90E-02	kg
Aluminum alloy, metal matrix composite {GLO}ǀ market for ǀ Alloc Rec, U	−1.31E-03	kg
Copper {RER}ǀ production, primary ǀ Alloc Rec, U	−1.11E-03	kg
Copper {GLO}ǀ market for ǀ Alloc Rec, U	−1.97E-04	kg
Aluminum alloy, metal matrix composite {GLO}ǀ market for ǀ Alloc Rec, U	−9.87E-03	kg
Electricity/Heat		
Electricity, medium voltage {IT}ǀ Electricity Production mixǀ Alloc Rec, U_RSE	8.00E-01	kWh
Emissions—Air		
Sulfur dioxide	4.80E-05	kg
Particulates, < 2.5 um	1.00E-04	kg
Particulates, > 10 um	1.04E-05	kg
Particulates, > 2.5 um, and < 10um	9.36E-05	kg
Emissions—Water		
Waste water	1.00E+00	kg
Sulfur dioxide	4.00E-02	kg
Chloride	4.00E-02	kg
Waste Treatment		
Waste plastic, mixture {Europe without Switzerland}ǀ treatment of waste plastic, mixture, municipal incineration ǀ Alloc Rec, U	6.99E-03	kg
Waste plastic, mixture {Europe without Switzerland}ǀ treatment of waste plastic, mixture, sanitary landfill ǀ Alloc Rec, U	5.92E-03	kg
Waste plastic, mixture {Europe without Switzerland}ǀ clinker production ǀ Alloc Rec, U	1.18E-02	kg

3 RESULTS

3.1 LCIA—Battery Production and End-of-Life

The life cycle environmental impacts associated with battery production and EoL phase of the three batteries described and broken down into key processes are reported in the following figures (LFP: Figure S6;

LFP with EoL: Figure S7; NMC 532: Figure S8; NMC 532 with EoL: Figure S9; NMC 622: Figure S10; and NMC 622 with EoL: Figure S11).

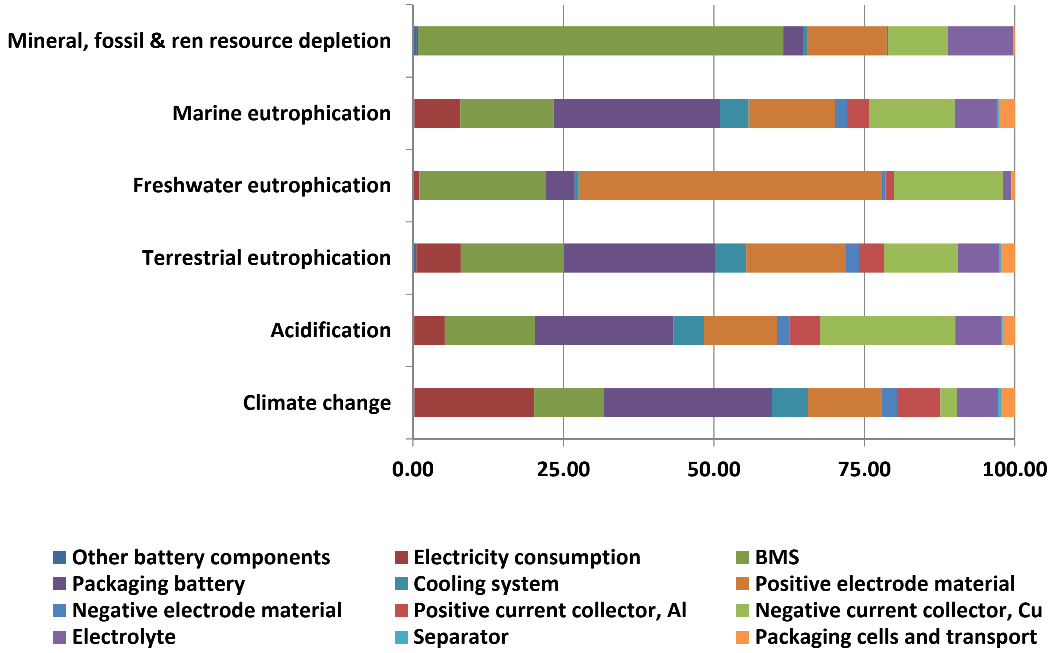

Figure S6. Life cycle impacts of LFP battery production broken down into key processes (other battery components like transport and metal refinery; electricity consumption including battery assembly and cell manufacturing)

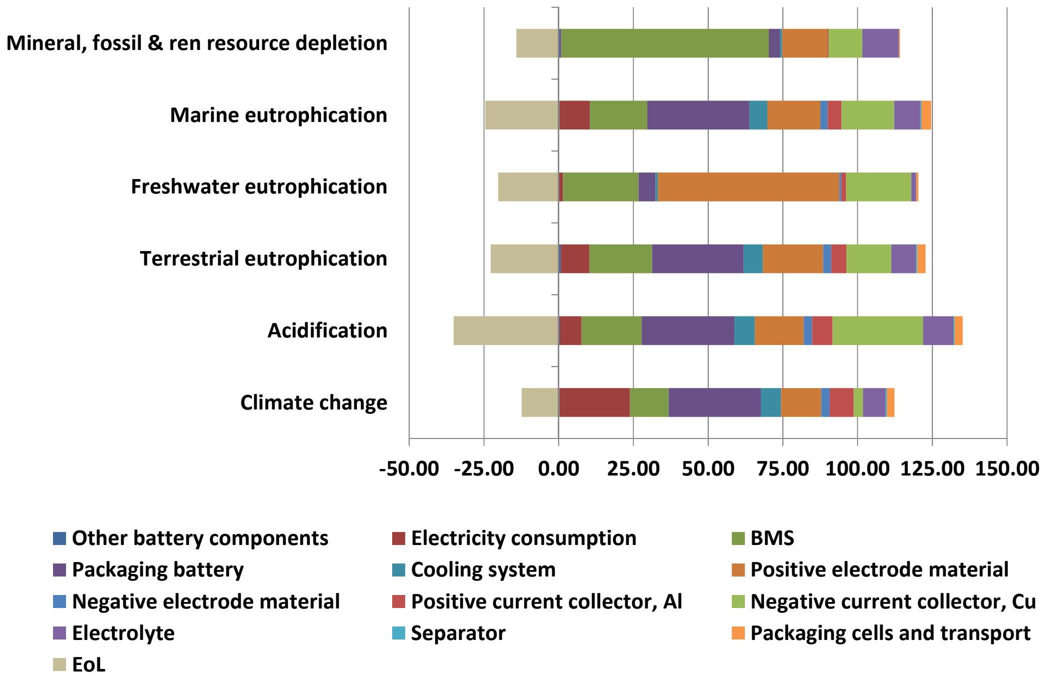

Figure S7. Life cycle impacts of LFP battery production and end-of-life (EoL) phase broken down into key processes (other battery components like transport and metal refinery; electricity consumption including battery assembly and cell manufacturing)

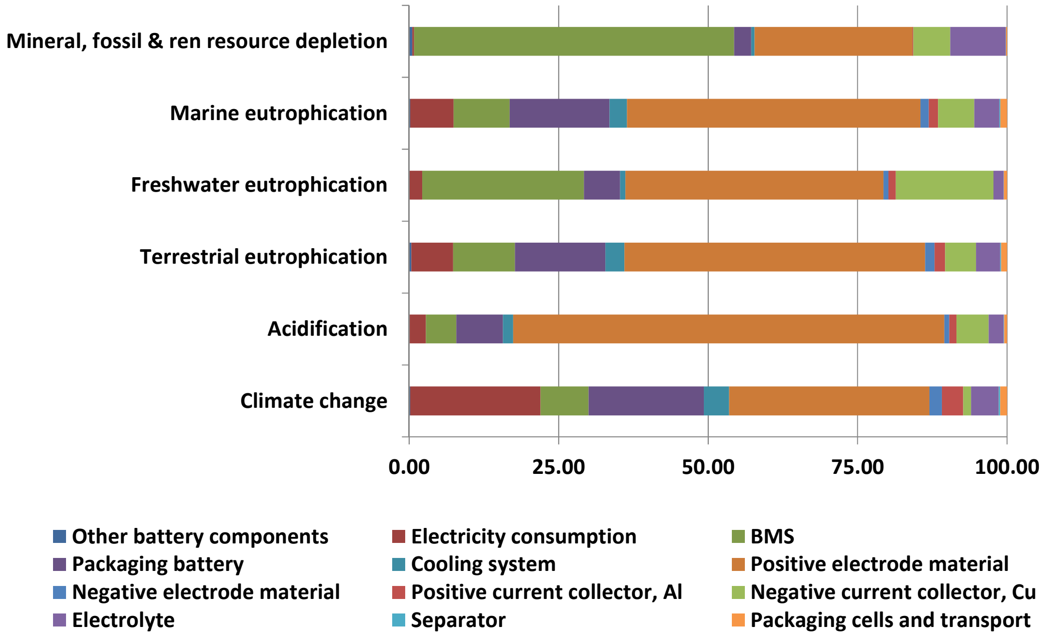

Figure S8. Life cycle impacts of NMC 532 battery production broken down into key processes (other battery components like transport and metal refinery; electricity consumption including battery assembly and cell manufacturing)

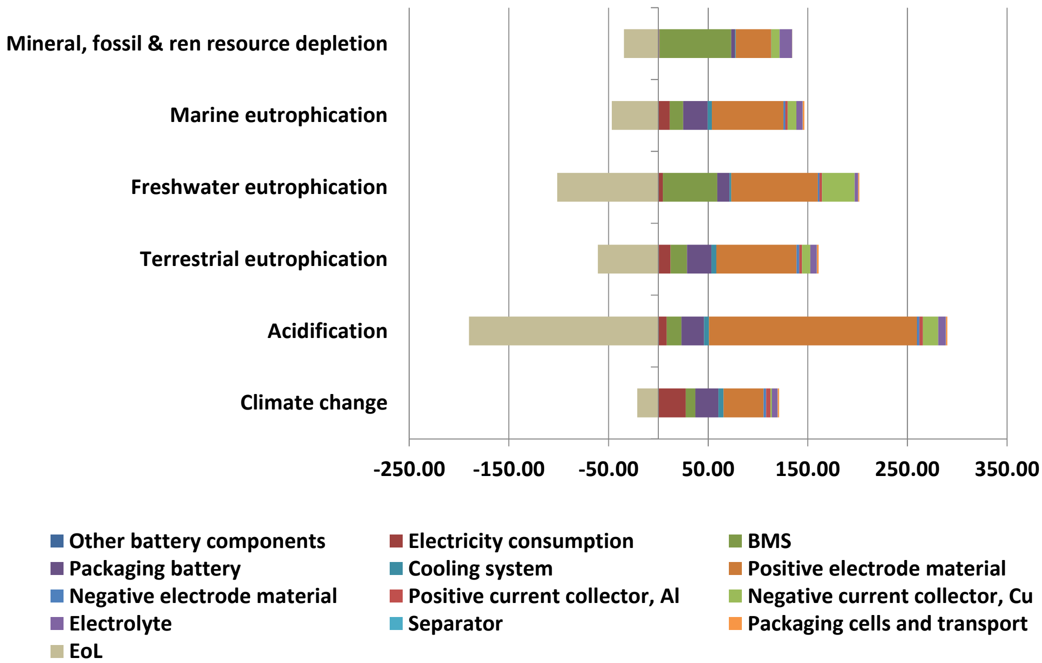

Figure S9. Life cycle impacts of NMC 532 battery production and end-of-life (EoL) phase broken down into key processes (other battery components like transport and metal refinery; electricity consumption including battery assembly and cell manufacturing)

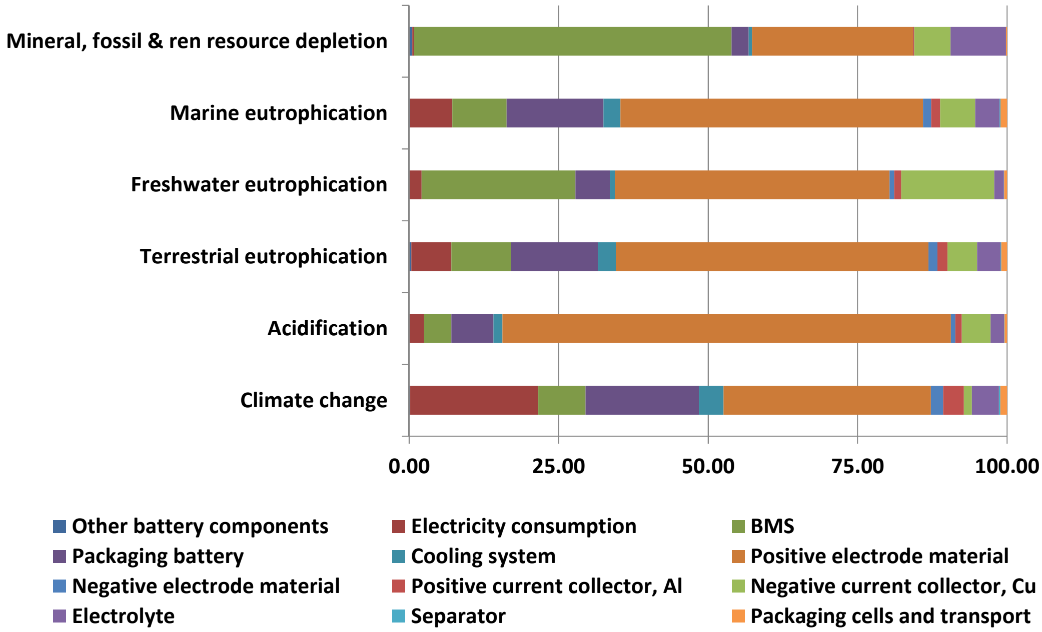

Figure S10. Life cycle impacts of NMC 622 battery production broken down into key processes (other battery components like transport and metal refinery; electricity consumption including battery assembly and cell manufacturing)

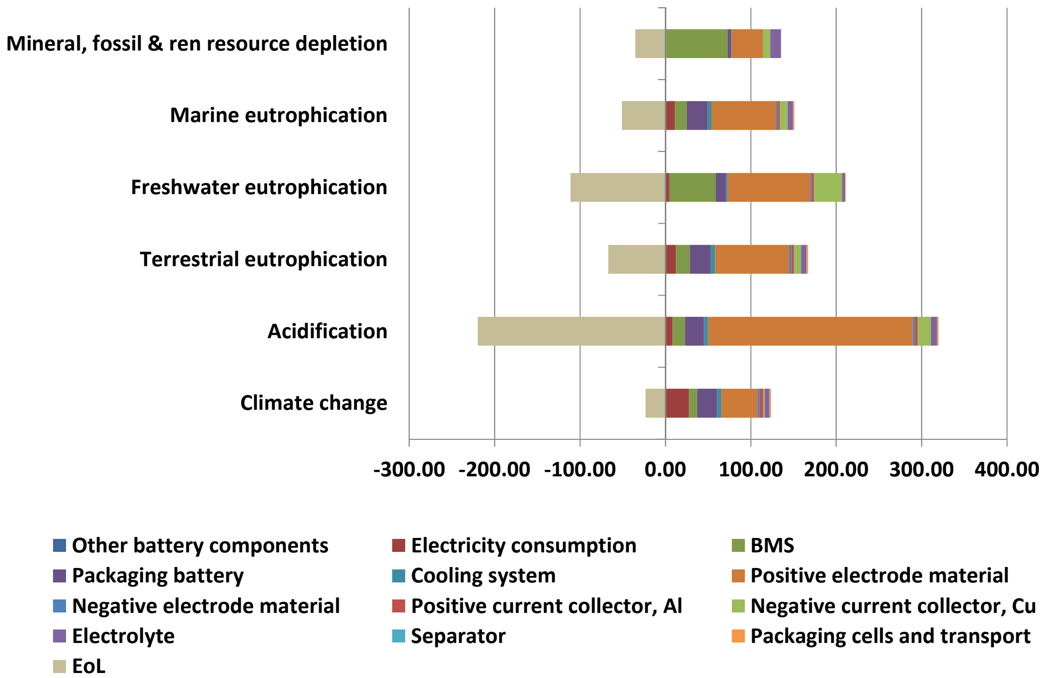

Figure S11. Life cycle impacts of NMC 622 battery production and end-of-life (EoL) phase broken down into key processes (other battery components like transport and metal refinery; electricity consumption including battery assembly and cell manufacturing)

3.2 Monte Carlo Analysis

A Monte Carlo analysis was carried out in order to quantify the uncertainty in the final results caused by the variability and uncertainty of secondary input data. The following tables present the estimated distribution of the LCA results, describing the mean value (MV), median value (MDV), standard deviation (SD), coefficient of variation (CV), and 95% confidence interval (the 2.5th percentile and the 97.5th percentile). Data refer to 1 kWh of battery capacity while considering EoL (Table S26) or not (

Table S27).

Table S26. Monte Carlo analysis simulation: main results. Data refers to 1 kWh of battery capacity while considering the end-of-life phase. MV: mean value; MDV: median value; SD: standard deviation; CV: coefficient of variation.

Battery	**Impact Category**	**Units**	**EoL**						
			MV	**MDV**	**SD**	**CV (%)**	**2.5%**	**97.5%**	**SEM**
LFP	Climate change	kg CO_2 eq	1.03E+02	1.03E+02	4.16E+00	4.05	9.56E+01	1.12E+02	1.32E-01
	Acidification	molc H+ eq	7.27E-01	7.22E-01	5.22E-02	7.19	6.40E-01	8.53E-01	1.65E-03
	Terrestrial eutrophication	molc N eq	1.02E+00	1.02E+00	7.53E-02	7.35	8.82E-01	1.19E+00	2.38E-03
	Freshwater eutrophication	kg P eq	1.11E-01	1.02E-01	4.91E-02	44.10	7.23E-02	2.04E-01	1.55E-03
	Marine eutrophication	kg N eq	1.29E-01	1.27E-01	1.49E-02	11.50	1.08E-01	1.65E-01	4.72E-04
	Mineral, fossil, and renewable resource depletion	kg Sb eq	7.19E-02	6.82E-02	2.03E-02	28.30	4.38E-02	1.22E-01	6.42E-04
NMC 532	Climate change	kg CO_2 eq	9.56E+01	9.51E+01	5.18E+00	5.42	8.72E+01	1.08E+02	1.64E-01
	Acidification	molc H+ eq	6.93E-01	6.86E-01	5.09E-02	7.34	6.11E-01	8.03E-01	1.61E-03
	Terrestrial eutrophication	molc N eq	9.03E-01	8.96E-01	6.47E-02	7.17	7.87E-01	1.05E+00	2.05E-03
	Freshwater eutrophication	kg P eq	6.50E-02	5.73E-02	3.08E-02	47.40	3.16E-02	1.55E-01	9.73E-04
	Marine eutrophication	kg N eq	1.18E-01	1.18E-01	1.13E-02	9.52	1.00E-01	1.45E-01	3.56E-04
	Mineral, fossil, and renewable resource depletion	kg Sb eq	4.84E-02	4.55E-02	1.42E-02	29.40	2.90E-02	8.39E-02	4.50E-04
NMC 622	Climate change	kg CO_2 eq	9.59E+01	9.52E+01	5.22E+00	5.45	8.75E+01	1.08E+02	1.65E-01
	Acidification	molc H+ eq	7.04E-01	6.99E-01	5.19E-02	7.37	6.21E-01	8.17E-01	1.64E-03
	Terrestrial eutrophication	molc N eq	9.05E-01	9.01E-01	6.66E-02	7.35	7.93E-01	1.05E+00	2.10E-03
	Freshwater eutrophication	kg P eq	6.76E-02	5.83E-02	5.61E-02	82.90	3.33E-02	1.45E-01	1.77E-03
	Marine eutrophication	kg N eq	1.18E-01	1.17E-01	1.16E-02	9.76	1.01E-01	1.46E-01	3.65E-04
	Mineral, fossil, and renewable resource depletion	kg Sb eq	4.83E-02	4.59E-02	1.37E-02	28.40	2.96E-02	8.21E-02	4.34E-04
		CED							
LFP	Non-renewable and biomass	MJ	1.07E+00	1.07E+00	9.86E-02	9.18E+00	8.99E-01	1.28E+00	3.12E-03
	Non-renewable and nuclear	MJ	1.48E+02	1.44E+02	3.57E+01	2.41E+01	9.19E+01	2.29E+02	1.13E+00
	Non-renewable and fossil	MJ	1.30E+03	1.29E+03	8.91E+01	6.87E+00	1.14E+03	1.49E+03	2.82E+00
	Renewable and biomass	MJ	5.31E+01	5.02E+01	1.12E+01	9.18	4.12E+01	7.87E+01	3.55E-01
	Renewable and water	MJ	1.27E+02	1.27E+02	4.44E+00	24.10	1.19E+02	1.36E+02	1.41E-01
	Renewable, wind, solar, and geothermal	MJ	4.10E+01	4.03E+01	3.68E+00	6.87	3.60E+01	4.99E+01	1.16E-01
NMC 532	Non-renewable and biomass	MJ	1.10E+00	1.10E+00	9.69E-02	21.20	9.33E-01	1.30E+00	3.07E-03
	Non-renewable and nuclear	MJ	1.33E+02	1.28E+02	3.18E+01	3.49	8.20E+01	2.03E+02	1.01E+00
	Non-renewable and fossil	MJ	1.30E+03	1.29E+03	1.00E+02	8.98	1.12E+03	1.51E+03	3.16E+00
	Renewable and biomass	MJ	5.05E+01	4.85E+01	8.45E+00	8.78	4.02E+01	7.08E+01	2.67E-01
	Renewable and water	MJ	1.12E+02	1.12E+02	3.93E+00	24.00	1.05E+02	1.20E+02	1.24E-01
	Renewable, wind, solar, and geothermal	MJ	4.30E+01	4.22E+01	4.03E+00	7.70	3.76E+01	5.37E+01	1.27E-01
NMC 622	Non-renewable and biomass	MJ	1.11E+00	1.11E+00	9.48E-02	16.70	9.34E-01	1.31E+00	3.00E-03
	Non-renewable and nuclear	MJ	1.33E+02	1.29E+02	3.29E+01	3.51	8.17E+01	2.12E+02	1.04E+00
	Non-renewable and fossil	MJ	1.30E+03	1.29E+03	1.07E+02	9.37	1.12E+03	1.54E+03	3.38E+00
	Renewable and biomass	MJ	5.11E+01	4.89E+01	9.54E+00	8.52	4.02E+01	7.40E+01	3.02E-01
	Renewable and water	MJ	1.12E+02	1.12E+02	3.94E+00	24.80	1.05E+02	1.20E+02	1.25E-01
	Renewable, wind, solar, and geothermal	MJ	4.31E+01	4.22E+01	4.11E+00	8.23	3.76E+01	5.33E+01	1.30E-01

Table S27. Monte Carlo analysis simulation: main results. Data refers to 1 kWh of battery capacity while not considering the end-of-life phase.

Battery	Impact Category	Units	No EoL						
			MV	MDV	SD	CV (%)	2.5%	97.5%	SEM
LFP	Climate change	kg CO_2 eq	1.14E+02	1.14E+02	4.75E+00	4.16	1.06E+02	1.25E+02	1.50E-01
	Acidification	molc H+ eq	9.80E-01	9.77E-01	6.35E-02	6.48	8.73E-01	1.13E+00	2.01E-03
	Terrestrial eutrophication	molc N eq	1.26E+00	1.25E+00	9.42E-02	7.50	1.10E+00	1.47E+00	2.98E-03
	Freshwater eutrophication	kg P eq	1.49E-01	1.31E-01	7.69E-02	51.60	9.35E-02	3.14E-01	2.43E-03
	Marine eutrophication	kg N eq	1.91E-01	1.86E-01	3.36E-02	17.60	1.46E-01	2.70E-01	1.06E-03
	Mineral, fossil, and renewable resource depletion	kg Sb eq	8.16E-02	7.79E-02	1.92E-02	23.50	5.38E-02	1.29E-01	6.07E-04
NMC 532	Climate change	kg CO_2 eq	1.15E+02	1.14E+02	5.29E+00	4.61	1.06E+02	1.26E+02	1.67E-01
	Acidification	molc H+ eq	2.01E+00	1.99E+00	6.57E-02	3.28	1.90E+00	2.16E+00	2.08E-03
	Terrestrial eutrophication	molc N eq	1.45E+00	1.44E+00	1.17E-01	8.02	1.25E+00	1.72E+00	3.68E-03
	Freshwater eutrophication	kg P eq	1.12E-01	9.86E-02	5.29E-02	47.10	6.09E-02	2.36E-01	1.67E-03
	Marine eutrophication	kg N eq	1.83E-01	1.80E-01	2.11E-02	11.50	1.50E-01	2.34E-01	6.66E-04
	Mineral, fossil, and renewable resource depletion	kg Sb eq	6.45E-02	6.20E-02	1.40E-02	21.70	4.49E-02	1.01E-01	4.43E-04
NMC 622	Climate change	kg CO_2 eq	1.17E+02	1.16E+02	5.69E+00	4.86	1.08E+02	1.30E+02	1.80E-01
	Acidification	molc H+ eq	2.24E+00	2.23E+00	7.99E-02	3.56	2.12E+00	2.41E+00	2.53E-03
	Terrestrial eutrophication	molc N eq	1.51E+00	1.49E+00	1.34E-01	8.89	1.29E+00	1.79E+00	4.23E-03
	Freshwater eutrophication	kg P eq	1.20E-01	1.00E-01	8.29E-02	69.20	6.26E-02	2.96E-01	2.62E-03
	Marine eutrophication	kg N eq	1.87E-01	1.84E-01	2.31E-02	12.30	1.53E-01	2.42E-01	7.29E-04
	Mineral, fossil, and renewable resource depletion	kg Sb eq	6.55E-02	6.23E-02	1.53E-02	23.30	4.62E-02	1.04E-01	4.83E-04
CED									
LFP	Non-renewable and biomass	MJ	1.02E+00	1.01E+00	8.92E-02	8.79	8.55E-01	1.22E+00	2.82E-03
	Non-renewable and nuclear	MJ	1.56E+02	1.53E+02	3.60E+01	23.10	9.78E+01	2.39E+02	1.14E+00
	Non-renewable and fossil	MJ	1.41E+03	1.41E+03	1.00E+02	7.08	1.23E+03	1.61E+03	3.16E+00
	Renewable and biomass	MJ	5.65E+01	5.36E+01	1.11E+01	19.70	4.46E+01	8.83E+01	3.52E-01
	Renewable and water	MJ	1.48E+02	1.47E+02	4.96E+00	3.36	1.38E+02	1.58E+02	1.57E-01
	Renewable, wind, solar, and geothermal	MJ	3.90E+01	3.84E+01	3.40E+00	8.71	3.45E+01	4.75E+01	1.08E-01
NMC 532	Non-renewable and biomass	MJ	1.08E+00	1.07E+00	9.78E-02	9.08	9.08E-01	1.29E+00	3.09E-03
	Non-renewable and nuclear	MJ	1.50E+02	1.45E+02	3.47E+01	23.10	9.43E+01	2.29E+02	1.10E+00
	Non-renewable and fossil	MJ	2.11E+03	2.09E+03	1.93E+02	8.79	1.75E+03	2.51E+03	6.10E+00
	Renewable and biomass	MJ	5.55E+01	5.32E+01	9.48E+00	23.10	4.42E+01	7.89E+01	3.00E-01
	Renewable and water	MJ	1.43E+02	1.43E+02	4.14E+00	7.08	1.36E+02	1.52E+02	1.31E-01
	Renewable, wind, solar, and geothermal	MJ	4.21E+01	4.15E+01	3.49E+00	19.70	3.74E+01	5.03E+01	1.10E-01
NMC 622	Non-renewable and biomass	MJ	1.08E+00	1.08E+00	9.62E-02	3.36	9.12E-01	1.28E+00	3.04E-03
	Non-renewable and nuclear	MJ	1.50E+02	1.45E+02	3.62E+01	8.71	9.37E+01	2.32E+02	1.15E+00
	Non-renewable and fossil	MJ	2.26E+03	2.23E+03	2.33E+02	9.08	1.85E+03	2.74E+03	7.36E+00
	Renewable and biomass	MJ	5.58E+01	5.38E+01	9.33E+00	23.10	4.45E+01	8.11E+01	2.95E-01
	Renewable and water	MJ	1.48E+02	1.47E+02	3.94E+00	9.16	1.40E+02	1.56E+02	1.25E-01
	Renewable, wind, solar, and geothermal	MJ	4.25E+01	4.18E+01	3.80E+00	17.10	3.77E+01	5.15E+01	1.20E-01

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