Sodium-ion batteries with $Ti_1Al_1TiC_{1.85}$ MXene as negative electrode: Life Cycle Assessment and Life Critical Resource Use Analysis

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Summary: This supporting information contains a full inventory of the different batteries components.

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1 SYSTEM DESCRIPTION: BATTERIES PRODUCTION AND ASSEMBLY

The production of each component and all the processes that refer to coin batteries production phase were modelled within SimaPro software. Datasets for Na-ion batteries are shown in Table S1.
Energy consumption related to battery coins construction and assembly phases was modelled by the low voltage Italian electricity mix, updated to 2019, as defined by [1][1]. Laboratory consumption was monitored through "smart plugs" connected to an energy consumption monitoring system. For equipment connected to the network with an industrial plug, the consumption estimations were assumed, measuring the intensity of the electric current, using an amperometric clamp.

Table S1. Dataset for the production of a Na-ion coin battery: Na_Laboratory (Na_Lab) and Na_Industrial (Na_Ind). The source of information used is mentioned in the name.

UF output	Na_Lab	Na_Ind	
Battery coin, Na-ion, lab RSE {IT}| production LAB | Alloc Rec, U_RSE	7.18	-	g
Battery coin, Na-ion, lab RSE {IT}| production Pil2 | Alloc Rec, U_RSE	-	6	g
Materials Input	**Na_Lab**	**Na_Ind**	
Cathode, $Na_{0.44}MnO_2$, for Na-Ion batteries LAB| Alloc Rec, U_RSE	0.0355	-	g
Cathode, $Na_{0.44}MnO_2$_noE_for Na-Ion batteries Pil2| Alloc Rec, U_RSE	-	0,0468	g
Anode, Mxene, for Na-Ion batteries | Alloc Rec, U_RSE	0.0191	-	g
Anode, Mxene_noE_for Na-Ion batteries Pil2 | Alloc Rec, U_RSE	-	0,0227	g
Electrolyte for Na-ion battery, NaPF6 {GLO}| production | Alloc Rec, U_Peters_RSE	1.1845	0,0217	g
Steel, low-alloyed {GLO}| market for | Alloc Rec, S	5.7695		g

[1] The work cited [1], refers to high voltage electricity mix production. For the transition from high to low voltage (the voltage level to which the laboratory equipment is connected), network losses of 5.6% were considered.

Styrene-butadiene rubber SBR {RER}| production | Alloc Rec, U_Peters_RSE	0.1405		g
Glass fibre {GLO} market for | Allo Rec, S	0.0268	-	g
Battery separator {GLO}|market for | Allo Rec, S	-	0.0004	g
Electricity/heat	**Na_Lab**	**Na_Ind**	
Electricity, low voltage {IT}| Electricity Production mix 2019 | Alloc Rec, U_RSE	-	0.002	kWh

For the industrial Lithium-ion battery (Li_Ind), a pouch cell (NMC type) from an automotive battery has been broken down and all the elements present inside have been classified (Figure S1).
Once components were catalogued, samples were taken and weight. Data was provided with reference to a 1 cm diameter disc of each assessed component: anode, cathode, and separator. Considering the battery design (coin), the active material was considered to be present only in one side of the charge carrier, and not in both sides as in the pouch configuration.

Datasets for Li_Ind coin battery are shown in Table S2.

Energy consumption related to battery construction and assembly phases was modelled by the low voltage Italian electricity mix, updated to 2019, as defined by [1][2].

Figure S1. Part of a lithium-ion automotive battery (and cell pouch)**.**

Table S2. Dataset for the production of a Li-ion coin battery; Li_Industrial (Li_Ind). The source of information used is mentioned in the name.

UF output		
Battery coin_EpouchLi_Li-ion NMC 532, lab RSE {IT}| production | Alloc Rec, U_RSE	6.11	g
Materials Input		
Positive electrode material for Li-Ion battery_NMC 532 | Alloc Rec, U_RSE_FAAM	0.0362	g
Electrode substrate for Li-ion battery_positive electrode| Alloc Rec, U_FAAM for COIN_RSE	0.0106	g
Negative carbonaceous electrode material for Li-Ion battery_NMC | Alloc Rec, U_FAAM_RSE	0.0232	g
Electrode substrate for Li-ion battery_negative electrode | Alloc Rec, U_FAAM_RSE	0.0182	g
Electrolyte for Li-ion battery, 1M LiPF6 {GLO}| production | Alloc Rec, U_Majeau-Bettez_RSE	0.0217	g
Battery separator {GLO}| market for | Alloc Rec, S	0.0004	g
Steel, low-alloyed {GLO}| market for | Alloc Rec, S	5.7695	g
Styrene-butadiene rubber SBR {RER}| production | Alloc Rec, U_Peters_RSE	0.1405	g
Electricity/heat		
Electricity, low voltage {IT}| Electricity Production mix 2019 | Alloc Rec, U_RSE	0.0011	kWh

[2] The work cited [1], refers to gross production. For the transition from high to low voltage (the voltage level to which the laboratory equipment is connected), network losses of 5.6% were considered.

2 LIFE CYCLE INVENTORY (LCI)

2.1 Electrodes

2.1.1 Cathode

2.1.1.1 Na batteries

The positive electrode (cathode) is covered with electro-chemically active materials, an aggregate (binder) and carbon black. The active material is $Na_{0.44}MnO_2$.
Binder is Polyvinylidene fluoride (PVDF), and the solvent is N-methylpyrrolidone (NMP). Solvent evaporates after application of electrode pastes to current collectors.
The production of the active material was modelled according to primary laboratory data.

Table S3. Dataset for the production of the positive electrode. The source of information used is mentioned in the name

UF output	Na_Lab	Na_Ind	
Cathode, $Na_{0.44}MnO_2$, for Na-Ion batteries LAB| Alloc Rec, U_RSE	0.0355	-	g
Cathode, $Na_{0.44}MnO_2$_noE_for Na-Ion batteries Pil2| Alloc Rec, U_RSE	-	0.0468	g
Materials Input	**Na_Lab**	**Na_Ind**	
Aluminium, wrought alloy {GLO}| market for | Alloc Rec, U	0.0140	0.0106	g
Sheet rolling, aluminium {GLO}| market for | Alloc Rec, U	0.0140	0.0106	g
Ink_$Na_{0.44}MnO_2$ active material, for Na-Ion batteries | Alloc Rec, U_RSE	0.0215	-	g
Ink_$Na_{0.44}MnO_2$ active material_noE_for Na-Ion batteries Pil2 | Alloc Rec, U_RSE	-	0.0362	g

Table S4. Dataset for the ink production step. The source of information used is mentioned in the name

UF output	Na_Lab	Na_Ind	
Ink_$Na_{0.44}MnO_2$ active material, for Na-Ion batteries | Alloc Rec, U_RSE	0.2		g
Ink_$Na_{0.44}MnO_2$ active material_noE_ for Na-Ion batteries Pil2 | Alloc Rec, U_RSE			
Materials Input	**Na_Lab**	**Na_Ind**	
$Na_{0.44}MnO_2$ active material, for Na-Ion batteries | Alloc Rec, U_RSE	0.160	-	g
$Na_{0.44}MnO_2$ active material_noE_for Na-Ion batteries | Alloc Rec, U_RSE	-	0.194	g
Polyvinylfluoride {GLO}| market for | Alloc Rec, U	0.02	0.003	g
Carbon black {GLO}| market for | Alloc Rec, U	0.02	0.003	g
N-methyl-2-pyrrolidone {GLO}| market for | Alloc Rec, U	0.721	0.213	g
Electricity/heat	**Na_Lab**	**Na_Ind**	
Electricity, low voltage {IT}| Electricity Production mix 2019 | Alloc Rec, U_RSE	0.5172	-	kWh
Emissions	**Na_Lab**	**Na_Ind**	
1-Methyl-2-pyrrolidinone	0.721	0.213	g

Table S5. Dataset for the production of the active material $Na_{0.44}Mn_{0.9}Cu_{0.1}O_2$. The source of information used is mentioned in the name.

UF output	Na_Lab	Na_Ind	
$Na_{0.44}MnO_2$ active material, for Na-Ion batteries | Alloc Rec, U_RSE	2	-	g
$Na_{0.44}MnO_2$ active material_noE_for Na-Ion batteries | Alloc Rec, U_RSE	-	2	g
Materials Input	**Na_Lab**	**Na_Ind**	
Sodium acetate {RER} | Alloc Rec, U_RSE (modelled according to [2])	0.744		g

Manganese acetate {RER}| production | Alloc Rec, U_RSE (modelled according to [3])	3.566		g
Citric acid {GLO}| market for | Alloc Rec, U	6.474		g
Water, deionised, from tap water, at user {Europe without Switzerland} | market for water, deionised, from tap water, at user | Alloc Rec, U	120		g
Electricity/heat	**Na_Lab**	**Na_Ind**	
Electricity, low voltage {IT}| Electricity Production mix 2019| Alloc Rec, U - RSE	0.13	-	kWh
Emissions	**Na_Lab**	**Na_Ind**	
Citric acid	6.474		g
Water	120		g

2.1.1.2 Li batteries

For the positive electrode, it was assumed the same inventory for the production of positive electrode (based on NMC 532) reported by [2].

2.1.2 Anode

2.1.2.1 Na batteries

The negative electrode (anode) is covered with electro-chemically active materials, an aggregate (binder) and carbon black. The active material is $Ti_1Al_1TiC_{1.85}$ MXene.
Binder is Polyvinylidene fluoride (PVDF), and the solvent is N-methylpyrrolidone (NMP). Solvent evaporates after application of electrode pastes to current collectors.
The production of the active material was modelled according to primary laboratory data.

Table S6. Dataset for the production of the negative electrode. The source of information used is mentioned in the name

UF output	**Na_Lab**	**Na_Ind**	
Anode, MXene, for Na-Ion batteries | Alloc Rec, U_RSE	0.0191	-	g
Anode, MXene_noE_for Na-Ion batteries Ind | Alloc Rec, U_RSE	-	0.0227	g
Materials Input	**Na_Lab**	**Na_Ind**	
Aluminium, wrought alloy {GLO}| market for | Alloc Rec, U	0.0140	0.0106	g
Sheet rolling, aluminium {GLO}| market for | Alloc Rec, U	0.0140	0.0106	g
Ink_Mxene active material, for Na-Ion batteries | Alloc Rec, U_RSE	0.0051	-	g
Ink_MXene active material_noE_for Na-Ion batteries Ind | Alloc Rec, U_RSE	-	0.0121	g

Table S7. Dataset for the ink production step. The source of information used is mentioned in the name

UF output	**Na_Lab**	**Na_Ind**	
Ink_MXene active material, for Na-Ion batteries | Alloc Rec, U_RSE	0.2		g
Ink_MXene active material_noE_for Na-Ion batteries Ind | Alloc Rec, U_RSE			
Materials Input	**Na_Lab**	**Na_Ind**	
MXene_after cleaning for Na-Ion batteries | Alloc Rec, U_RSE	0.16		g
MXene_after cleaning_noE_for Na-Ion batteries Pil | Alloc Rec, U_RSE	-	0.194	g
Polyvinylfluoride {GLO}| market for | Alloc Rec, U	0.02	0.003	g
Carbon black {GLO}| market for | Alloc Rec, U	0.02	0.003	g
N-methyl-2-pyrrolidone {GLO}| market for | Alloc Rec, U	0.721	0.213	g
Electricity/heat	**Na_Lab**	**Na_Ind**	
Electricity, low voltage {IT}| Electricity Production mix 2019| Alloc Rec, U - RSE	0.52	-	kWh
Emissions	**Na_Lab**	**Na_Ind**	

1-Methyl-2-pyrrolidinone	0.721	0.213	g

Table S8. Dataset for the production of MXene: after cleaning process. The source of information used is mentioned in the name

UF output	**Na_Lab**	**Na_Ind**	
MXene_after cleaning, for Na-Ion batteries | Alloc Rec, U_RSE	3		g
MXene_after cleaning_noE_for Na-Ion batteries Pil | Alloc Rec, U_RSE			
Materials Input	**Na_Lab**	**Na_Ind**	
MAXphase sintering, for Na-Ion batteries | Alloc Rec, U_RSE	3	-	g
MAXphase sintering_noE_for Na-Ion batteries | Alloc Rec, U_RSE	-	3	g
Hydrogen fluoride {GLO}| market for | Alloc Rec, U	11.88	1.018	g
Water, deionised, from tap water, at user {Europe without Switzerland}| market for water, deionised, from tap water, at user | Alloc Rec, U	1028.1	1039	g
Emissions	**Na_Lab**	**Na_Ind**	
Water	1028.1	1039	g
Hydrogen fluoride	11.88	1.018	g

Table S9. Dataset for the production of MAXphase: sintering process. The source of information used is mentioned in the name

UF output	**Na_Lab**	**Na_Ind**	
MAXphase sintering, for Na-Ion batteries | Alloc Rec, U_RSE	12	-	g
MAXphase sintering_noE_for Na-Ion batteries | Alloc Rec, U_RSE	-	12	g
Materials Input	**Na_Lab**	**Na_Ind**	
$Ti_1Al_1TiC_{1.85}$ active material, for Na-Ion batteries | Alloc Rec, U_RSE	12	-	g
$Ti_1Al_1TiC_{1.85}$ active material_noE_for Na-Ion batteries | Alloc Rec, U_RSE	-	12	
Graphite {RER}| production | Alloc Rec, U	15	15	g
Graphite, battery grade {GLO}| market for | Alloc Rec, U	3	3	g
Boron nitride BN {GLO}| market for | Alloc Rec, U_RSE	0.75	0.75	g
Electricity/heat	**Na_Lab**	**Na_Ind**	
Electricity, low voltage {IT}| Electricity Production mix 2019 | Alloc Rec, U_RSE	7.6	-	kWh

Table S10. Dataset for the $Ti_1Al_1TiC_{1.85}$ active material production. The source of information used is mentioned in the name

UF output	**Na_Lab**	**Na_Ind**	
$Ti_1Al_1TiC_{1.85}$ active material, for Na-Ion batteries | Alloc Rec, U_RSE	40.09		g
$Ti_1Al_1TiC_{1.85}$ active material_noE_for Na-Ion batteries | Alloc Rec, U_RSE			
Materials Input	**Na_Lab**	**Na_Ind**	
Titanium, primary {GLO}| market for | Alloc Rec, U	10.31		g
Aluminium, primary {GLO}| market for | Alloc Rec, U	5.81		g
Titanium carbide, Tic {RER}| production | Alloc Rec, U_RSE	23.9		g
Electricity/heat	**Na_Lab**	**Na_Ind**	
Electricity, low voltage {IT}| Electricity Production mix 2019| Alloc Rec, U_RSE	0.4	-	kWh

Boron nitride (BN) production was modelled in the Simapro considering the following chemical reaction (boric acid with urea):

$$2H_3BO_3 + CO(NH_2)_2 = 2BN + CO_2 + 5H_2O \quad \text{Eq. 1}$$

Table S11. Dataset for the boron nitride production. The source of information used is mentioned in the name

UF output		
Boron nitride BN {GLO}| market for | Alloc Rec, U_RSE	1	kg
Materials Input		
Boric acid, anhydrous, power {GLO}| market fir | Alloc Rec, U	2.491	kg
Urea, as N {RER}| production | Alloc Rec, U	1.210	kg
Emissions		
Carbon dioxide	0.887	kg
Water	1.815	kg

Titanium carbide production was modelled in the Simapro considering the following chemical reaction, where titanium dioxide reacts with carbon at high temperature (2000 ° C):

$$TiO_2 + 3C = TiC + 2CO \quad \text{Eq. 2}$$

Table S12. Dataset for the boron nitride production. The source of information used is mentioned in the name

UF output		
Titanium carbide, TiC {RER}| production | Alloc Rec, U_RSE	1	kg
Materials Input		
Chemical factory, organics {GLO}| market for | Alloc Rec, U	4E-10	p
Titanium dioxide {RER}| market for | Alloc Rec, U	1.333815	kg
Electricity/heat		
Coke {GLO}| market for | Alloc Rec, U	19.3	MJ
Electricity, medium voltage {RER}| market group for | Alloc Rec, U	3.1	kWh
Emissions		
Methane, fossil	0.00148	kg
Carbon monoxide, fossil	0.935577	kg
Hydrogen	0.00388	kg
Carbon dioxide, fossil	0.0122	kg

2.1.2.2 Li batteries

For the negative electrode, it was assumed the same inventory for the production of negative electrode reported by [2].

2.1.2.3 Separator

The separator role is to prevent electrodes (anode and cathode) from touching, while electrons flow in the electrolyte with as little resistance as possible.
For Na batteries:

- Na laboratory: the separator is a whatman microfiber filter (*i.e.*, glass fiber), the Ecoinvent dataset *Glass fiber {GLO} market for | Allo Rec, S* was used as a proxy.
- Na Industrial: it was assumed the same reported by Peters et al [5] for Na batteries *Battery separator {GLO} | market for | Allo Rec, S*.

For the Li battery, it was assumed the same separator as reported by Majeau-Bettez et al. [3].

2.1.2.4 Electrolyte

Na batteries

The electrolyte is made of sodium salts ($NaPF_6$) in a mixture of carbonate solvents. It was considered the same inventory reported by Peters et al [5].

Li battery

The electrolyte is made of lithium salt ($LiPF_6$) and solvents. In this study, it was assumed the inventory for the production of electrolyte reported by Ellingsen et al. [7].

2.1.2.5 Cell container

The cell container is a coin type that consists of a lower case (positive pole), an upper case (negative pole), a disk and a spring. All steel components were modelled in SimaPro considering the Ecoinvent dataset: *Steel low-alloyed {GLO} | market for | Alloc Rec, S*. For the gasket, the *Styrene-butadiene rubber SBR {RER} | production | Alloc Rec, U_Peters_RSE* dataset was considered.

3 RESULTS

3.1 LCIA – Sankey diagrams

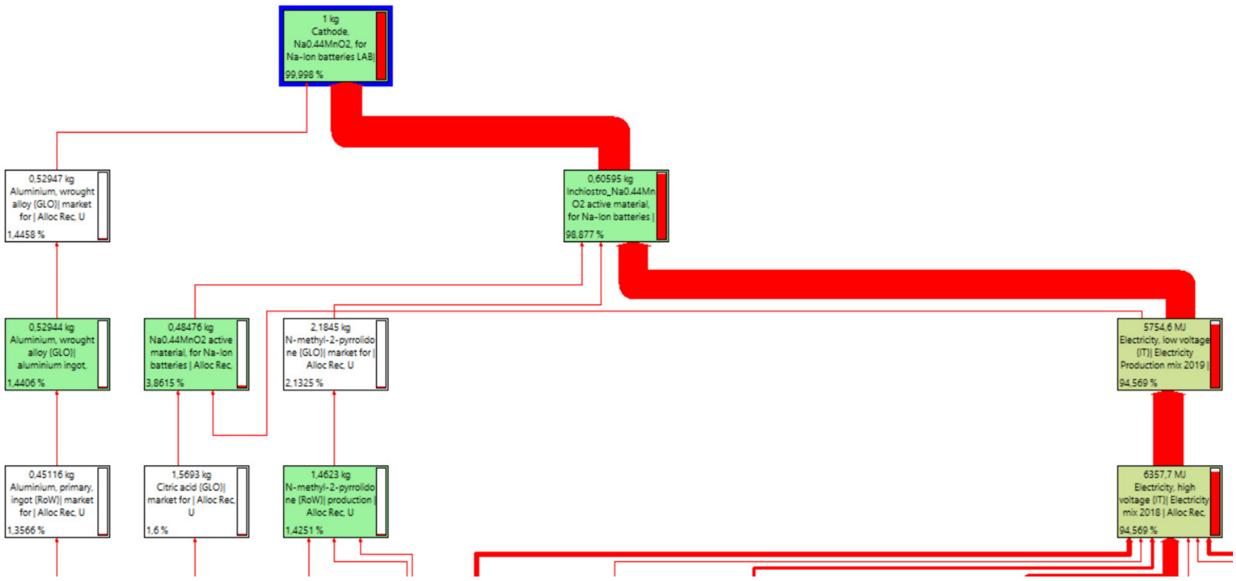

Figure S2. Na-ion laboratory coin battery: Sankey diagram for Climate Change impact category, expressed in %, for the production of 1 kg of $Na_{0,44}MnO_2$ cathode.

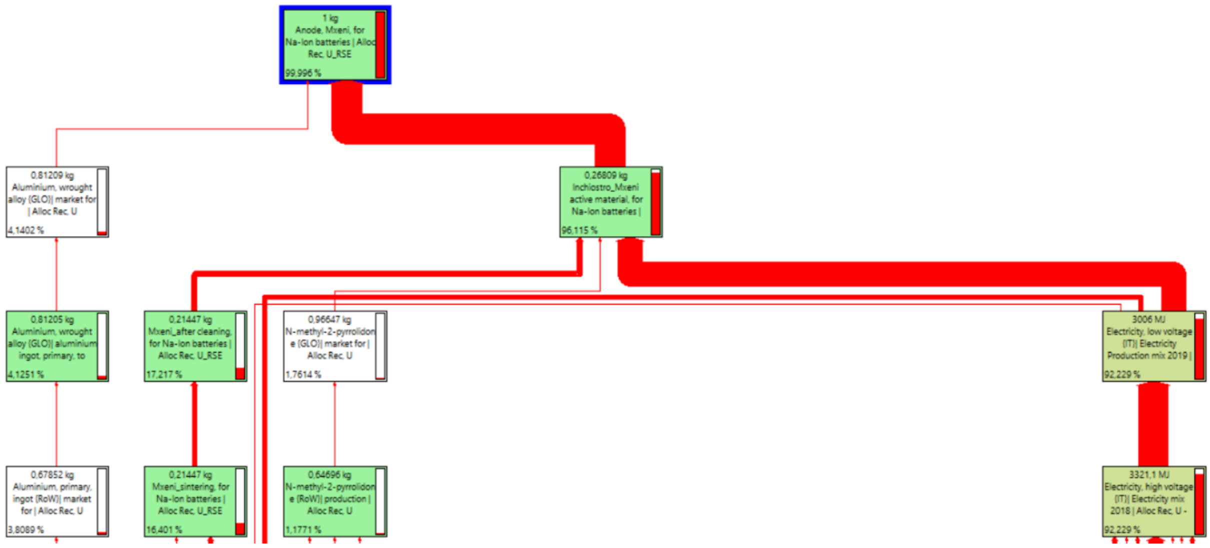

Figure S3. Na-ion laboratory coin battery: Sankey diagram for Climate Change impact category, expressed in %, for the production of 1 kg of anode.

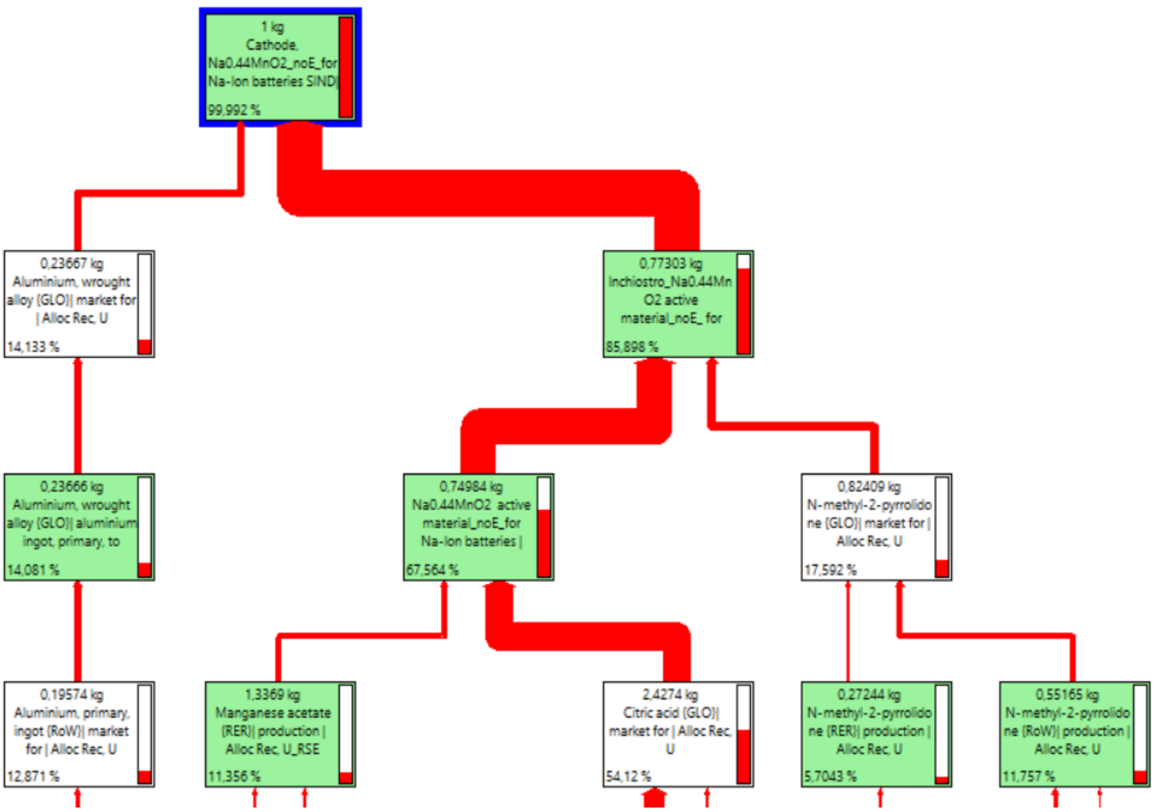

Figure S4. Na-ion industrial coin battery: Sankey diagrams for Climate Change impact category, expressed in %, for the production of 1 kg of $Na_{0,44}MnO_2$ cathode.

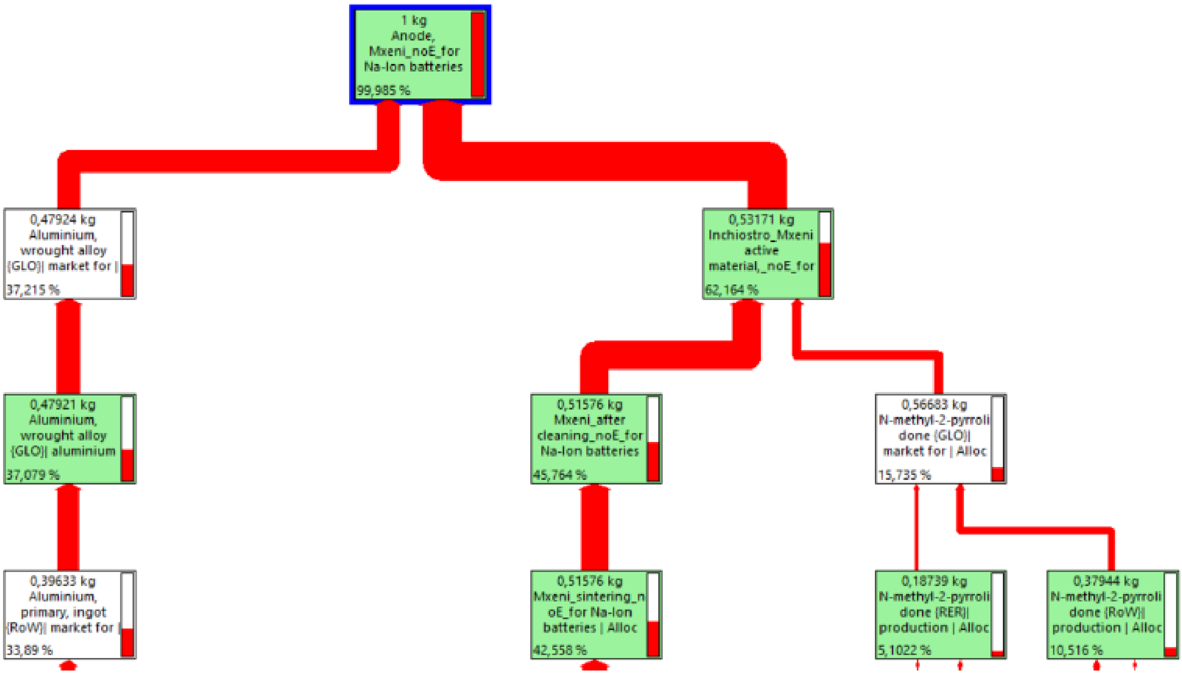

Figure S5. Na-ion industrial coin battery: Sankey diagrams for Climate Change impact category, expressed in %, for the production of 1 kg of anode.

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