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1. DATA FOR THE LAB-SCALE PROCESSES

On the Lab-Scale, the foreground system is split into the following, three different production steps:

[i] synthesis of **Li-containing materials** ($LiCoO_2$ and $LiMnPO_4$ respectively),

[ii] production of **composite** material, and finally

[iii] production of **electrode**, i.e. by applying the composite material on an aluminium foil in order to form the complete cathode.

Main data source for these foreground processes are the practical experiments executed by the authors at University of Fribourg concerning the synthesis of these various materials; and additional, mainly literature data in order to cover specific points/questions for all those situations, where the analysis of the experiments did not result in detailed enough information. From Table S.1 to Table S.3, the values from these practical experiments are summarized, together with their respective translation into an LCA language.

Table S.1 **Input and output data for the production of $LiCoO_2$ via the various, here examined pathways**

Material	Unit	amount						Remarks
		meth	eth	iso	t-but	phen	mix	
(i) Inputs								
Lithium alkoxide[1]	kg	1.300	3.938	2.434	2.882	4.713	3.225	
Cobalt chloride	kg	1.478	1.642	1.602	1.565	1.529	1.494	
Tetrahydrofuran[2]	kg	14.326	15.918	15.534	24.270	23.712	23.179	Density 0.889 kg/L
Methanol[2]	kg	3.573	-	-	-	-	-	Density 0.792 kg/L
Argon (gaseous)	kg	5.563	6.181	6.033	5.891	5.755	5.626	Density 1.669 kg/m^{3}
Nitrogen (liquid)	kg	361	401	391	382	373	365	Density 0.812 kg/L
Water, deionised	kg	278	309	301	294	287	281	
Electricity	kWh	90.6	96.7	103	109.2	110.1	125.3	
(ii) Outputs								
Lithium cobalt oxide	kg	1						Product
Lithium chloride	kg	0.956	2.674	1.036	1.012	0.995	0.973	Co-product[3]
Solvent, to recycling	kg	59.356	53.242	51.959	82.120	80.232	78.429	
Waste for disposal	kg	0.144	0.272	0.241	0.212	0.184	0.180	
Carbon dioxide, to air	kg	1.444	6.543	4.819	6.235	12.414	7.865	
Tetrahydrofuran, to air	kg	1.667	1.852	1.807	1.765	3.333	3.258	
Methanol, to air	kg	1.046	-	-	-	-	-	

[1] meth: lithium methoxide pathway (default assumption for modelling) / eth: lithium ethoxide pathway / iso: lithium isopropoxide pathway / t-but: lithium *tert*-butoxide pathway / phen: lithium phenoxide pathway / mix: pathway with mixture of Li tert-butoxide and Li phenoxide

[2] reported here is the amount, taking into account the recycled proportion of THF resp. methanol (i.e. the value represents each time those part that can't be recycled, and thus is actually "consumed" in the production process)

[3] For the default calculation on the lab-scale level, lithium chloride has been considered as by-product, i.e. all the impacts have been allocated to $LiCoO_2$ (i.e. a conservative approach is chosen like this).

A sensitivity calculation, using a mass-based allocation of all inputs and outputs results for the default pathway (i.e. pathway using lithium methoxide as starting material) in a reduction of the impacts by a factor of 4; due to the high amount of LiCl produced simultaneously in the examined chemical process – and this independent from the impact category.

Table S.2   Input and output data for the production of LiMnPO$_4$

Material	Unit	amount	Remarks
(i) Inputs			
Lithium hydroxide	kg	0.378	
Manganese acetate	kg	1.103	
Phosphoric acid	kg	0.473	Density 1.89 kg/L
Benzyl ether	kg	18.096	Density 1.04 kg/L
Hexane	kg	18.995	Density 0.655 kg/L
Trichloromethane	kg	16.193	Density 1.489 kg/L
Oleic acid	kg	0.412	Density 0.895 kg/L
Oleylamine	kg	3.006	Density 0.813 kg/L
Water (cooling)	m^3	38	
Electricity	kWh	1'314	
(ii) Outputs			
LiMnPO$_4$	kg	1	Product
Solvents, to recycling	kg	195.5	
Water, to river	m^3	38	
Wastes for disposal	kg	0.030	
Acetic acid, to air	kg	0.719	Stoichiometric amount

Table S.3   Input and output data for the production of the composite and the electrode materials, out of the Li-containing materials (LiCoO$_2$ resp. LiMnPO$_4$)

Material	Unit	composite material	electrode material	Remarks
(i) Inputs				
Li-containing material	kg	0.833		
Composite material	kg		0.857	
Carbon (SFG)	kg	0.168		
PVDF	kg		0.071	
NMP	kg		0.736	Density 1.03 kg/L
SP Carbon	kg		0.071	
Electricity	kWh	63.3	7.665	
(ii) Outputs				
Composite material	kg	1		Product
Electrode material	kg		1	Product
Wastes for disposal	kg	0.001	0.1	
NMP, to air	kg		0.736	

Carbon (SFG): name for graphite provided by the producer
PVDF: Polyvinylidenfluoride
NMP: N-Methyl-2-pyrrolidon
SP Carbon: name for the carbon black provided by the producer

2. DATA FOR THE (FUTURE) PILOT PRODUCTION

Starting point for the up-scaled inventory data of the two different Li-containing materials are the above listed lab-scale data from the experiments at the University of Fribourg. In Table S.4 and Table S.5 on the next two pages, the resulting values for a (future) pilot production are reported, together with a short description how these numbers have been derived from the lab-scale data. For $LiCoO_2$, the pathway with lithium methoxide as starting material is used here – due to economic reasons (this pathway has the lowest costs) this seems to be the most promising option among the pathways for the $LiCoO_2$ production examined on the Lab-scale.

Table S.4   Input and output data for the pilot production of LiCoO$_2$ (via the methoxide pathway)

Material	Unit	Upscaling High	Upscaling Low	Derivation of / Assumptions for upscaled data
(i) Inputs				
Lithium methoxide	kg	1.202	1.158	Assumed is a yield of 85% (**high**) and 90% (**low**) for Chloride consumption in overall process; and based on this a yield of 90% (**high**) and 95% (**low**) is assumed for lithium methoxide and 95% (**high**) and 98% (**low**) for CoCl$_2$ (in accordance with the modelling of chemical production processes reported in Hischier et al., 2005)
Cobalt chloride	kg	1.396	1.354	
Tetrahydrofuran	kg	0.025	0.012	Due to the "closed" system (as a batch process is assumed), the total THF amount is reduced to 20% (**high**) and 10% (**low**) compared to lab-scale process – and thereof, it is assumed that 2.5% are lost (and need to be replaced as an input); while the remaining 97.5% are recovered by an (internal) distillation process. Furthermore, it is assumed that THF is in large parts replaced by Methanol (MeOH) – i.e. we assume here that 90% of THF are replaced, and only 10% are still consumed in form of THF.
Methanol	kg	0.284	0.142	In addition to the above-mentioned amount of 90% of the THF, the MeOH input from the lab-scale process is (due to assumed "closed" system with a batch process) reduced to 10% compared to the lab-scale process – and from this total again 2.5% are lost (and need to be replaced as an input); while the remaining 97.5% are recovered by an (internal) distillation process.
Argon	kg	-		100% replaced by gaseous nitrogen
Nitrogen (gaseous)	kg	1.950	1.560	Assumption: use of 40% of Ar amount (in m^3) in Lab-Scale process
Nitrogen (liquid)	kg	-		Not needed anymore (i.e. 100% reduction)
Water, deionised	kg	55.6		Assumption: 80% less than in the Lab-Scale process
Electricity	kWh	45.678	18.271	**Low:** calculated, based on the procedure described in Piccinno et al., 2016 – the calculation details are shown below this table. **High:** Assumed is a 2.5 times higher consumption than calculated for the "low" scenario
Heat (from natural gas)	MJ	1.041	0.991	Energy amount for the distillation of the recovered amount of tetrahydrofuran and methanol – calculated according to procedure in Wampfler et al., 2010.
(ii) Outputs				
Lithium cobalt oxide	kg	1.0		Main product (reference value for all other values)
Lithium chloride	kg	0.775	0.796	Considered as a co-product. For the amount, a yield of 85% (**high**) and 90% (**low**) for chloride consumption in the overall process is assumed here.
Solvents, to recycling	kg	-		No external solvent recycling anymore (replaced by internal distillation processes – shown via the heat energy consumption above)
Wastes for disposal	kg	0.317	0.218	Assumption: 100% of remaining lithium methoxide and cobalt chloride
Carbon dioxide, to air	kg	1.349		Assumption: 3 mol CO$_2$/mol LiCoO$_2$, according to input from the University of Fribourg
Tetrahydrofuran, to air	kg	0.025	0.012	All losses (i.e. the above input) as emission to air
Methanol, to air	kg	0.284	0.142	All losses (i.e. the above input) as emission to air
Nitrogen, to air	kg	1.950	1.560	100% emitted to air

Calculation procedure (Piccinno et al., 2016) for estimation of the electricity consumption:

(i) HEATING

Specific heat capacity	C_p	1.72	J/g/K	Cp of the main solvent used (i.e. THF)
Mass of reaction mixture	m_{mix}	13.691	kg	sum of input materials & solvents (i.e. Li-Methoxide, $CoCl_2$, THF, methanol)
Reaction temperature	T	339.15	K	equal to 66°C (heating temperature in the upscaling process according to JP. Brog)
Reaction time	t	1	hour	process needs to be kept on this temperature for whole reaction time

--> HEATING ENERGY INPUT	Q_{heat}	1.937	MJ

(ii) MIXING

Density of reaction mixture	p_{mix}	0.839	kg/L	calculated from individual substances
		[kg/L]	[kg]	(data listed below)
Li-methoxide		0.6	1.182	
Cobalt chloride		3.356	1.396	
THF		0.889	0.988	
Methanol		0.79	10.124	
Reaction time	t	1	hour	

-->MIXING ENERGY INPUT	Q_{stir}	0.054	MJ

(iii) VACUUM PUMP

No approxmiation procedure in Piccino et al.
-> Data from LAB SCALE used ... assuming a 75% lower consumption

--> VACUUM PUMP ENERGY INPUT	Q_{vac}	16.497	MJ

(iv) FURNACE 1 (= HEATING)

Specific heat capacity	C_p	1.72	J/g/K	Cp of the main solvent used (i.e. THF)
Mass of reaction mixture	m_{mix}	13.691	kg	sum of input materials & solvents (see step i)
Reaction temperature	T	723.15	K	equal to 450°C (heating temperature for Furnace (I) according to JP. Brog)
Reaction time	t	1	hour	process needs to be kept on this temperature for whole reaction time

--> HEATING ENERGY INPUT	Q_{heat}	20.082	MJ

(v) CENTRIFUGE

--> HEATING ENERGY INPUT	Q_{cent}	0.036	MJ	10 kWh/t as maximum value

(iv) FURNACE 2 (= HEATING)

Specific heat capacity	C_p	1.72	J/g/K	Cp of the main solvent used (i.e. THF)
Mass of reaction mixture	m_{mix}	13.691	kg	sum of input materials & solvents (see step i)
Reaction temperature	T	873.15	K	equal to 600°C (heating temperature for Furnace (I) according to JP. Brog)
Reaction time	t	1	hour	process needs to be kept on this temperature for whole reaction time

--> HEATING ENERGY INPUT	Q_{heat}	27.170	MJ

--> TOTAL ENERGY CONSUMPTION		65.776	MJ
	resp.	18.271	kWh

Table S.5   Input and output data for the pilot production of LiMnPO₄

Material	Unit	Upscaling		Derivation of / Assumptions for upscaled data
		High	Low	
(i) Inputs				
Lithium hydroxide	kg	0.170	0.161	**High:** Assumption is a yield of 90% within the reaction equation for all three starting materials
Manganese acetate	kg	1.226	1.161	**Low**: Assumption is a yield of 95% within the reaction equation for all three starting materials (in accordance with the modelling of chemical production processes; reported in Hischier et al., 2005)
Phosphoric acid	kg	0.694	0.658	
Benzyl ether	kg	0.312	0.156	Assuming a "closed" system (as a batch process is assumed), the solvent consumption equals 20% (**high**) and 10% (**low**) compared to the lab-scale – in each case thereof, 2.5% are lost in internal solvent recovery process (i.e. distillation process to separate the various substances …) and need to be replaced as input
Hexane	kg	0.328	0.164	
Trichloromethane	kg	0.279	0.140	
Oleic acid	kg	0.007	0.004	
Oleylamine	kg	0.052	0.026	
Water, for cooling	m³	15		Assumption: 60% less than in the lab-scale process
Electricity	kWh	12.885	5.154	**Low:** calculated, based on the procedure described in Piccinno et al., 2016 – the calculation details are shown below this table. **High:** Assumed is a 2.5 times higher consumption than calculated for the "low" scenario
Heat (from natural gas)	MJ	20.866	10.433	Energy amount for the distillation of the recovered amount of solvents (i.e. benzyl ether, hexane, trichloro-methane, oleic acid, oleylamine), calculated according to procedure in Wampfler et al., 2010.
(ii) Outputs				
LiMnPO₄	kg	1.0		Main product (reference value for all other values)
Acetic acid	kg	0.808	0.766	A recovered amount – from the solvent recovery process – of 95% is assumed here (via condensation process), considered as by-product
Solvents, to recycling	kg	-		No external solvent recycling anymore (replaced by internal distillation)
Wastes for disposal	kg	0.209	0.099	Assumption: 100% of remaining input (i.e. lithium hydroxide, manganese acetate and phosphoric acid)
Acetic acid, to air	kg	0.043	0.040	Remaining 5% are losses in the solvent recovery process, assumed to be released to air
Benzyl ether, to air	kg	0.312	0.156	Losses (i.e. the above input amount) represent the amount that is no recovered in the solvent recovery process; assumed here to be released to air
Hexane, to air	kg	0.328	0.164	
Trichloromethane, to air	kg	0.279	0.140	
Oleic acid, to air	kg	0.007	0.004	
Oleylamine, to air	kg	0.052	0.026	
PO₃⁴⁻, to water	kg	0.067	0.032	Remaining amount assumed to be released to water
Water, to river	m³	15		Cooling water: 100% back to environment

Calculation procedure (Piccinno et al., 2016) for estimation of the electricity consumption:

(i) HEATING

Specific heat capacity	C_p	1.557	J/g/K	Cp of the main solvent used (here 1:1 mix of benzyl ether and hexane !)
Mass of reaction mixture	m_{mix}	2.468	kg	sum of input materials & solvents
Reaction temperature	T	553.15	K	equal to 280°C (heating temperature according to input from NH. Kwon)
Reaction time	t	2.5	hour	process needs to be kept on this temperature for whole reaction time

--> HEATING ENERGY INPUT $\boxed{Q_{heat} \quad 11.414 \qquad MJ}$

(ii) CENTRIFUGE (= Mixing, as process goes over a long period of 3.5 hours)

Density of reaction mixture	p_{mix}	1.495	kg/L	calculated from individual substances
		[kg/L]	[kg]	(data listed below)
Lithium hydroxide		1.46	0.161	
Manganese acetate		1.74	1.161	
Phosphoric acid		1.89	0.658	
Benzyl ether		1.047	0.156	
Hexane		0.6606	0.164	
Trichloromethane		1.49	0.140	
Oleic acid		0.894	0.004	
Oleylamine		0.828	0.026	
Reaction time	t	3.5	hour	

-->MIXING ENERGY INPUT $\boxed{Q_{stir} \quad 0.339 \qquad MJ}$

(iii) LIGAND EXCHANGE (= HEATING)

Specific heat capacity	C_p	1.557	J/g/K	Cp of the main solvent used (see step i)
Mass of reaction mixture	m_{mix}	2.468	kg	sum of input materials & solvents (see step i)
Reaction temperature	T	353.15	K	equal to 80°C (heating temperature according to input from NH. Kwon)
Reaction time	t	6	hour	process needs to be kept on this temperature for whole reaction time

--> HEATING ENERGY INPUT $\boxed{Q_{heat} \quad 5.514 \qquad MJ}$

(iv) DRYING (= HEATING)

Specific heat capacity	C_p	1.557	J/g/K	Cp of the main solvent used (see step i)
Mass of reaction mixture	m_{mix}	2.468	kg	sum of input materials & solvents (see step i)
Reaction temperature	T	333.15	K	equal to 60°C (input NH. Kwon)
Reaction time	t	2	hour	process needs to be kept on this temperature for whole reaction time

--> HEATING ENERGY INPUT $\boxed{Q_{heat} \quad 1.289 \qquad MJ}$

--> TOTAL ENERGY CONSUMPTION $\boxed{\begin{array}{ccc} & 18.556 & MJ \\ resp. & 5.154 & kWh \end{array}}$

3. (BACKGROUND) LIFE CYCLE INVENTORY DATASETS

3.1. Benzyl ether

Benzyl ether (($C_6H_5CH_2$)$_2$O, CAS-No. 103-50-4) is at room temperature a colourless to pale-yellow liquid with a boiling point around 298°C (see e.g. www.chemicalbook.com). According to Joshi et al., 1999, there exists several different routes for the synthesis of benzyl ether. The most conventional among these processes is the so-called "Wiliamson's synthesis", i.e. the reaction of benzyl chloride with sodium benzylate ($NaOCH_2Ph$) – reaction that has however been adapted by Joshi et al., 1999, to the following reaction equation, which is modelled here:

$$2 \ (C_6H_5)CH_2Cl + 2 \ NaOH \ \text{-->} \ (C_6H_5)CH_2)_2O + 2 \ NaCl + H_2O$$
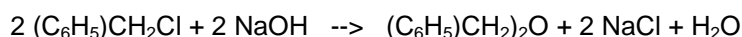
The whole process is modelled here in accordance with the modelling principle for "weak documented chemicals" from Hischier et al., 2005. An overall efficiency of the process of 99% as reported in Joshi et al., 1999, is assumed here – and the amount of the various starting materials is calculated, based on this yield. Heat, electricity, compressed air, nitrogen and water consumption values, as well as transport efforts and infrastructure are modelled with default values (according to procedure in Hischier et al., 2005 – using updated values, collected and calculated by the ecoinvent Centre, 2017). Table S.6 summarizes the resulting input and output values, used to calculate the production of 1 kg of benzyl ether.

Table S.6   Input and output data for the production of 1 kg of benzyl ether

[per kg Benzyl Ether]		Total	Remark
INPUTS			
Benzyl chloride	kg	1.29E+00	stoechiometric calc., 99% yield
Sodium hydroxide	kg	4.08E-01	stoechiometric calc., 99% yield
Electricity, medium voltage	kWh	0.416	default estimation
heat, in chemical industry	MJ	2.35	default estimation
nitrogen	kg	0.019	default estimation
compressed air, 1000 kPa gauge	m3	0.5	default estimation
tap water	kg	2.60E-02	default estimation
Water, cooling, unspecified natural origin	m3	1.64E-02	default estimation
Water, river	m3	8.60E-04	default estimation
Water, well, in ground	m3	8.30E-04	default estimation
Chemical plant, organics	unit	4.00E-10	default estimation
Transport, by train	tkm	1.02E+00	standard distances & means
Transport, by lorry	tkm	1.70E-01	standard distances & means
OUTPUTS			
benzyl ether	kg	1	
wastewater, average	m3	2.70E-06	default estimation
nitrogen, to air	kg	1.90E-02	default estimation
water, to air	m3	1.40E-03	default estimation
Benzyl chloride, to air	kg	2.58E-03	0.2% of input
Carbon dioxide, fossil, to air	kg	2.26E-02	from waste water treatment
water, to water	m3	1.67E-02	default estimation
Benzyl chloride, to water	kg	1.03E-03	calculated from mass balances
Sodium ions, to water	kg	2.32E-01	calculated from mass balances
Chloride ions, to water	kg	3.60E-01	calculated from mass balances
COD, BOD	kg	5.48E-03	calculated from water emissions
TOC, DOC	kg	1.71E-03	calculated from water emissions

For the emission side, 0.2% of the input amount of benzyl chloride is assumed to be "emitted to air" while the remaining part goes as part of the waste water flow into the waste water treatment plant (WWTP). There, 90% of this amount is digested and transformed into carbon dioxide (emitted into air) and chloride respectively, the latter leaving the system in their ionic form as a respective release into water. The remaining 10% pass the WWTP and thus are accounted as the release of benzyl chloride into water. All the produced NaCl is assumed to leave the system as release to the water – while sodium hydroxide on the input side is added in excess quantities, assuming a complete (material) recovery of the non-reacting part. According to the description in Hischier et al., 2005, COD, BOD, TOC and DOC values are estimated from the releases in the treated waste water. For their calculation, a worst-case scenario of BOD = COD and TOC = DOC was used.

3.2. Cobalt chloride

According to Wikipedia (Wikipedia Contributors, 2015), cobalt(II) chloride is an inorganic compound of cobalt and chlorine, with the formula $CoCl_2$. It is usually supplied as the hexahydrate $CoCl_2 \bullet 6H_2O$, one of the most commonly used cobalt compounds in the lab. The hexahydrate is deep purple in colour, whereas the anhydrous form is sky blue. Cobalt chloride has been classified as a substance of very high concern by the European Chemicals Agency (ECA) as it is a suspected carcinogen. According to the information given in Majeau-Bettez et al., 2011, cobalt chloride is produced out of cobalt hydroxide according to the following stoichiometric equation:

$$Co(OH)_2 + 2\ HCl\ \rightarrow\ CoCl_2 \bullet 6(H_2O)$$
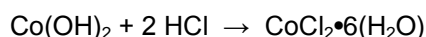
Also in this case, the whole process is modelled in accordance with the modelling principle for "weak documented chemicals" from Hischier et al., 2005, i.e. an overall efficiency of the process of 95% is assumed – and the amount of starting materials is calculated, based on this yield. Heat, electricity, compressed air, nitrogen and water consumption values, as well as transport efforts and infrastructure are modelled with default values (according to procedure in Hischier et al., 2005 – using updated values, collected and calculated by the ecoinvent Centre, 2017). For the emission side, 0.2% of the two starting materials are assumed to be emitted to air, the remaining part goes as part of the waste water flow into the waste water treatment plant (WWTP) like described in Hischier et al., 2005. There, cobalt ions are bound to 50% in the sludge, while the other 50% are released to nature. The Cl-ions are assumed to be released from the WWTP to 100% in their ionic form. Table S.7 summarizes the resulting input and output values, used to calculate the production of 1 kg of cobalt chloride.

Table S.7   Input and output data for the production of 1 kg of cobalt chloride

[per kg Cobalt Chloride]		Total	Remark
INPUTS			
Cobalt hydroxide	kg	7.54E-01	stoechiometric calc., 95% yield
Hydrochloric acid	kg	5.91E-01	stoechiometric calc., 95% yield
Electricity, medium voltage	kWh	0.416	default estimation
heat, in chemical industry	MJ	2.35	default estimation
nitrogen	kg	0.019	default estimation
compressed air, 1000 kPa gauge	m3	0.5	default estimation
tap water	kg	2.60E-02	default estimation
Water, cooling, unspecified natural origin	m3	1.64E-02	default estimation
Water, river	m3	8.60E-04	default estimation
Water, well, in ground	m3	8.30E-04	default estimation
Chemical plant, organics	unit	4.00E-10	default estimation
Transport, by train	tkm	8.07E-01	standard distances & means
Transport, by lorry	tkm	1.34E-01	standard distances & means
OUTPUTS			
Cobalt chloride, at plant	kg	1	
wastewater, average	m3	2.70E-06	default estimation
nitrogen, to air	kg	1.90E-02	default estimation
water, to air	m3	1.40E-03	default estimation
Cobalt hydroxide, to air	kg	1.51E-03	0.2% of input
Hydrochloric acid, to air	kg	1.18E-03	0.2% of input
water, to water	m3	1.67E-02	default estimation
Cobalt ions, to water	kg	1.15E-02	calculated from mass balances
Chloride ions, to water	kg	2.76E-02	calculated from mass balances

3.3. Cobalt hydroxide

Cobalt hydroxide, the starting material used in the production of cobalt chloride has to be modelled in a similar way due to the fact that a dataset for this substance doesn't exist neither in the database. According to Majeau-Bettez et al., 2011, cobalt hydroxide could be produced out of cobalt sulphate:

$$CoSO_4 + 2\ NaOH \rightarrow Co(OH)_2 + Na_2SO_4$$
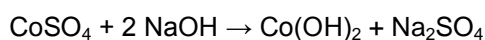
Again, the entire process is modelled according to the modelling principle for "weak documented chemicals" reported in Hischier et al., 2005, i.e. an overall efficiency of the process of 95% is assumed – and the amount of starting materials is calculated, based on this yield. Heat, electricity, compressed air, nitrogen and water consumption values, as well as transport efforts and infrastructure are modelled with default values (according to procedure in Hischier et al., 2005 – using updated values, collected and calculated by the ecoinvent Centre, 2017). For the emission side, 0.2% of the cobalt-containing starting material is assumed to be emitted to air, the remaining part goes as part of the waste water flow into the waste water treatment plant (WWTP). There, cobalt ions are bound to 50% in the sludge, while the other 50% are released to nature. The sulphate ions are assumed to be released from the WWTP to 100% in their ionic form. The excess sodium hydroxide goes 100% to the WWTP, and leaves in its ionic form (i.e. as sodium ions) the plant in the release to (river) water.

The Table S.8 summarizes the resulting input and output values, used to calculate the production of 1 kg of cobalt hydroxide.
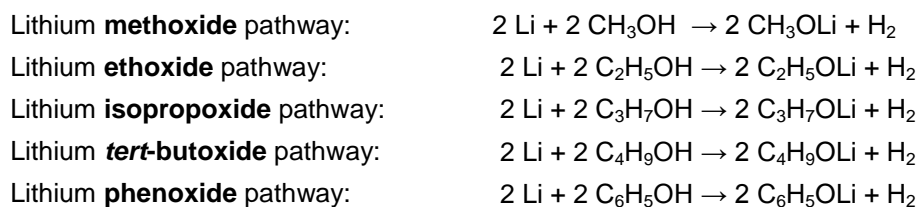
Table S.8   **Input and output data for the production of 1 kg of cobalt hydroxide**

[per kg Cobalt Hydroxide]		Total	Remark
INPUTS			
Cobalt Sulphate	kg	1.76E+00	stoechiometric calc., 95% yield
Sodium hydroxide	kg	9.06E-01	stoechiometric calc., 95% yield
Electricity, medium voltage	kWh	0.416	default estimation
heat, in chemical industry	MJ	2.35	default estimation
nitrogen	kg	0.019	default estimation
compressed air, 1000 kPa gauge	m3	0.5	default estimation
tap water	kg	2.60E-02	default estimation
Water, cooling, unspecified natural origin	m3	1.64E-02	default estimation
Water, river	m3	8.60E-04	default estimation
Water, well, in ground	m3	8.30E-04	default estimation
Chemical plant, organics	unit	4.00E-10	default estimation
Transport, by train	tkm	1.60E+00	standard distances & means
Transport, by lorry	tkm	2.66E-01	standard distances & means
OUTPUTS			
Cobalt hydroxide, at plant	kg	1	
wastewater, average	m3	2.70E-06	default estimation
nitrogen, to air	kg	1.90E-02	default estimation
water, to air	m3	1.40E-03	default estimation
Cobalt sulphate, to air	kg	3.51E-03	0.2% of input
water, to water	m3	1.67E-02	default estimation
Sodium, to water	kg	2.60E-02	calculated from mass balances
Cobalt ions, to water	kg	1.60E-02	calculated from mass balances
Sulphate, to water	kg	5.22E-02	calculated from mass balances

3.4. Lithium alkoxides and aryloxides

According to Bradley et al., 2001, and Turova et al., 2002, alkoxides are conjugate bases of an alcohol and consist of an organic group bonded to a negatively charged oxygen atom. They can be written as RO−, where R is the organic substituent. Alkoxides are strong bases and, when R is not bulky, good nucleophiles and good ligands. Alkoxides can be produced by several routes starting from an alcohol. Highly reducing metals react directly with alcohols to give the corresponding metal alkoxide.

The formation reactions for the different types of lithium alkoxides and lithium aryloxides taken into account here are the following:

Lithium **methoxide** pathway:	$2\,Li + 2\,CH_3OH \rightarrow 2\,CH_3OLi + H_2$
Lithium **ethoxide** pathway:	$2\,Li + 2\,C_2H_5OH \rightarrow 2\,C_2H_5OLi + H_2$
Lithium **isopropoxide** pathway:	$2\,Li + 2\,C_3H_7OH \rightarrow 2\,C_3H_7OLi + H_2$
Lithium ***tert*-butoxide** pathway:	$2\,Li + 2\,C_4H_9OH \rightarrow 2\,C_4H_9OLi + H_2$
Lithium **phenoxide** pathway:	$2\,Li + 2\,C_6H_5OH \rightarrow 2\,C_6H_5OLi + H_2$

Again, all processes are modelled with the support of the modelling principle for "weak documented chemicals" reported in Hischier et al., 2005. For the above reactions, an overall efficiency of the process of 90%, as reported in the process description published in Talalaeva et al., 1964, is used here. The amount of the various starting materials is then calculated based on this yield. Heat, electricity, compressed air, nitrogen and water consumption values, as well as transport efforts and infrastructure are modelled with default values (according to procedure in Hischier et al., 2005 – using

updated values, collected and calculated by the ecoinvent Centre, 2017). Concerning the emissions and releases, all excess lithium is assumed to leave the system in ionic form as release into water (i.e. to pass via the WWTP). From the various (starting) alcohols 0.2% of the initial amounts are assumed to be emitted to air, the remaining part goes as part of the waste water flow into the waste water treatment plant (WWTP) like described in Hischier et al., 2005. There, 90% of this amount is digested and transformed into carbon dioxide (emitted into air). The remaining 10% pass the WWTP and thus are accounted as release of the respective alcohol into water. According to the description in Hischier et al., 2005, COD, BOD, TOC and DOC values are estimated from the releases in the treated waste water. For their calculation, a worst-case scenario of BOD = COD and TOC = DOC was used. Table S.9 to Table S.13 summarize the resulting input and output values, used to calculate the production of 1 kg of the various lithium alkoxides and lithium aryloxides taken into account here.

Table S.9   Input and output data for the production of 1 kg of lithium methoxide

[per kg Lithium methoxide]		Total	Remark
INPUTS			
Lithium	kg	2.03E-01	stoechiometric calc., 90% yield
Methanol	kg	9.38E-01	stoechiometric calc., 90% yield
Electricity, medium voltage	kWh	0.416	default estimation
heat, in chemical industry	MJ	2.35	default estimation
nitrogen	kg	0.019	default estimation
compressed air, 1000 kPa gauge	m3	0.5	default estimation
tap water	kg	2.60E-02	default estimation
Water, cooling, unspecified natural origin	m3	1.64E-02	default estimation
Water, river	m3	8.60E-04	default estimation
Water, well, in ground	m3	8.30E-04	default estimation
Chemical plant, organics	unit	4.00E-10	default estimation
Transport, by train	tkm	6.84E-01	standard distances & means
Transport, by lorry	tkm	1.14E-01	standard distances & means
OUTPUTS			
Lithium methoxide, at plant	kg	1	
wastewater, average	m3	2.70E-06	default estimation
nitrogen, to air	kg	1.90E-02	default estimation
water, to air	m3	1.40E-03	default estimation
Methanol, to air	kg	1.88E-03	0.2% of input
Carbon dioxide, to air	kg	1.14E-01	from waste water treatment
water, to water	m3	1.67E-02	default estimation
Methanol, to water	kg	9.19E-03	calculated from mass balances
Lithium ion, to water	kg	2.03E-02	calculated from mass balances
COD, BOD	kg	1.32E-02	calculated from water emissions
TOC, DOC	kg	3.44E-03	calculated from water emissions

Table S.10   Input and output data for the production of 1 kg of lithium ethoxide

[per kg Lithium ethoxide]		Total	Remark
INPUTS			
Lithium	kg	1.48E-01	stoechiometric calc., 90% yield
Ethanol	kg	9.84E-01	stoechiometric calc., 90% yield
Electricity, medium voltage	kWh	0.416	default estimation
heat, in chemical industry	MJ	2.35	default estimation
nitrogen	kg	0.019	default estimation
compressed air, 1000 kPa gauge	m3	0.5	default estimation
tap water	kg	2.60E-02	default estimation
Water, cooling, unspecified natural origin	m3	1.64E-02	default estimation
Water, river	m3	8.60E-04	default estimation
Water, well, in ground	m3	8.30E-04	default estimation
Chemical plant, organics	unit	4.00E-10	default estimation
Transport, by train	tkm	6.80E-01	standard distances & means
Transport, by lorry	tkm	1.13E-01	standard distances & means
OUTPUTS			
Lithium ethoxide, at plant	kg	1	
wastewater, average	m3	2.70E-06	default estimation
nitrogen, to air	kg	1.90E-02	default estimation
water, to air	m3	1.40E-03	default estimation
Ethanol, to air	kg	1.97E-03	0.2% of input
Carbon dioxide, to air	kg	1.66E-01	from waste water treatment
water, to water	m3	1.67E-02	default estimation
Ethanol, to water	kg	9.65E-03	calculated from mass balances
Lithium ion, to water	kg	1.48E-02	calculated from mass balances
COD, BOD	kg	1.93E-02	calculated from water emissions
TOC, DOC	kg	5.03E-03	calculated from water emissions

Table S.11   Input and output data for the production of 1 kg of lithium isopropoxide

[per kg Lithium isopropoxide]		Total	Remark
INPUTS			
Lithium	kg	1.17E-01	stoechiometric calc., 90% yield
Isopropanol	kg	1.01E+00	stoechiometric calc., 90% yield
Electricity, medium voltage	kWh	0.416	default estimation
heat, in chemical industry	MJ	2.35	default estimation
nitrogen	kg	0.019	default estimation
compressed air, 1000 kPa gauge	m3	0.5	default estimation
tap water	kg	2.60E-02	default estimation
Water, cooling, unspecified natural origin	m3	1.64E-02	default estimation
Water, river	m3	8.60E-04	default estimation
Water, well, in ground	m3	8.30E-04	default estimation
Chemical plant, organics	unit	4.00E-10	default estimation
Transport, by train	tkm	6.77E-01	standard distances & means
Transport, by lorry	tkm	1.13E-01	standard distances & means
OUTPUTS			
Lithium isopropoxide, at plant	kg	1	
wastewater, average	m3	2.70E-06	default estimation
nitrogen, to air	kg	1.90E-02	default estimation
water, to air	m3	1.40E-03	default estimation
Isopropanol, to air	kg	2.02E-03	0.2% of input
Carbon dioxide, to air	kg	1.96E-01	from waste water treatment
water, to water	m3	1.67E-02	default estimation
Isopropanol, to water	kg	9.91E-03	calculated from mass balances
Lithium ion, to water	kg	1.17E-02	calculated from mass balances
COD, BOD	kg	2.28E-02	calculated from water emissions
TOC, DOC	kg	5.94E-03	calculated from water emissions

Table S.12   Input and output data for the production of 1 kg of lithium *tert*-butoxide

[per kg Lithium tert-butoxide]		Total	Remark
INPUTS			
Lithium	kg	9.63E-02	stoechiometric calc., 90% yield
Tert-butanol	kg	1.03E+00	stoechiometric calc., 90% yield
Electricity, medium voltage	kWh	0.416	default estimation
heat, in chemical industry	MJ	2.35	default estimation
nitrogen	kg	0.019	default estimation
compressed air, 1000 kPa gauge	m3	0.5	default estimation
tap water	kg	2.60E-02	default estimation
Water, cooling, unspecified natural origin	m3	1.64E-02	default estimation
Water, river	m3	8.60E-04	default estimation
Water, well, in ground	m3	8.30E-04	default estimation
Chemical plant, organics	unit	4.00E-10	default estimation
Transport, by train	tkm	6.75E-01	standard distances & means
Transport, by lorry	tkm	1.13E-01	standard distances & means
OUTPUTS			
Lithium tert-butoxide, at plant	kg	1	
wastewater, average	m3	2.70E-06	default estimation
nitrogen, to air	kg	1.90E-02	default estimation
water, to air	m3	1.40E-03	default estimation
Tert-butanol, to air	kg	2.06E-03	0.2% of input
Carbon dioxide, to air	kg	2.16E-01	from waste water treatment
water, to water	m3	1.67E-02	default estimation
Tert-butanol, to water	kg	1.01E-02	calculated from mass balances
Lithium ion, to water	kg	9.63E-03	calculated from mass balances
COD, BOD	kg	2.51E-02	calculated from water emissions
TOC, DOC	kg	6.53E-03	calculated from water emissions

Table S.13   Input and output data for the production of 1 kg of lithium phenoxide

[per kg Lithium phenoxide]		Total	Remark
INPUTS			
Lithium	kg	7.71E-02	stoechiometric calc., 90% yield
Phenol	kg	1.05E+00	stoechiometric calc., 90% yield
Electricity, medium voltage	kWh	0.416	default estimation
heat, in chemical industry	MJ	2.35	default estimation
nitrogen	kg	0.019	default estimation
compressed air, 1000 kPa gauge	m3	0.5	default estimation
tap water	kg	2.60E-02	default estimation
Water, cooling, unspecified natural origin	m3	1.64E-02	default estimation
Water, river	m3	8.60E-04	default estimation
Water, well, in ground	m3	8.30E-04	default estimation
Chemical plant, organics	unit	4.00E-10	default estimation
Transport, by train	tkm	6.73E-01	standard distances & means
Transport, by lorry	tkm	1.12E-01	standard distances & means
OUTPUTS			
Lithium tert-butoxide, at plant	kg	1	
wastewater, average	m3	2.70E-06	default estimation
nitrogen, to air	kg	1.90E-02	default estimation
water, to air	m3	1.40E-03	default estimation
Phenol, to air	kg	2.09E-03	0.2% of input
Carbon dioxide, to air	kg	2.59E-01	from waste water treatment
water, to water	m3	1.67E-02	default estimation
Phenol, to water	kg	1.02E-02	calculated from mass balances
Lithium ion, to water	kg	7.71E-03	calculated from mass balances
COD, BOD	kg	2.33E-02	calculated from water emissions
TOC, DOC	kg	7.81E-03	calculated from water emissions

3.5. Oleylamine

According to the respective Toxic Substance Control Act (TSCA) annex (US-EPA, 1986) Oleylamine, or 9-octadecenylamine (ODA, CAS No. 112-90-3) is a yellow liquid with an ammoniacal odour. It has very low volatility and water solubility although water is soluble in it. It is miscible with a variety of organic solvents. Within this project, ODA has been synthesised by the authors in the following way:

- To a 5-litre flange neck flask fitted with overhead stirrer, temperature probe, nitrogen inlet and a 500 cm^3 dropping funnel was charged oleic acid (400 g, 1.416 mol) and dichloromethane (3.20 L). The resultant solution was heated to reflux (39-41°C) and thionyl chloride (202.4 g, 1.2 eq.) added over 10 minutes between 39-41°C.

- The reaction mixture was heated at reflux for 3 hours, sampling the mixture at hourly intervals (sample quenched into anhydrous methanol, shaken well, and stored at ambient for >1 hour before submitted to analytical development for analysis). The reaction was shown to be 99.9% complete after 3 hours. As the reaction mixture was used in the subsequent amidation reaction without delay, no isomerisation to the trans-isomer was observed.

- To a 20-litre flange-neck flask fitted with overhead stirrer, nitrogen inlet, condenser (with silica drying tube) and a gas sparging inlet was charged dichloromethane (12.00 Kg, ~9.1 L). The solvent was cooled to 0-10 °C and then ammonia (960 g) was charged as a gas via the sparging inlet over 140 minutes, maintaining the reaction mixture between 0-10°C. The acid chloride solution in dichloromethane was then added to the stirred ammonia solution via transfer line and

500 cm3 dropping funnel over 32 minutes, maintaining the reaction temperature below 20°C. The resultant pink-coloured suspension could be stirred at ambient temperature overnight. A sample was taken (sample quenched into methanol). The resulting reaction mixture was shown to be 76.69% oleylamide and 22.53% oleic acid.

For the calculations here, dichloromethane and thionyl chloride are assumed to have a catalytic role (i.e. don't react during the above described procedure) and therefore, the above described process is simplified here with the stoichiometric equation:

$$C_{18}H_{34}O_2 \text{ (Oleic acid)} + NH_3 \rightarrow C_{18}H_{35}NH_2 + O_2$$

Again, this process is modelled here according to the modelling principle for "weak documented chemicals" reported in Hischier et al., 2005, using the above reported efficiency for the oleic acid transformation of 77%. For the further inputs, the default yield of 95% is used in order to calculate the related input amounts. Heat, electricity, compressed air, nitrogen and water consumption values, as well as transport efforts and infrastructure are modelled with default values (according to procedure in Hischier et al., 2005 – using updated values, collected and calculated by the ecoinvent Centre, 2017).

Table S.14   Input and output data for the production of 1 kg of oleylamine

[per kg Oleylamine]		Total	Remark
INPUTS			
Oleic acid	kg	1.09E+00	stoechiometric calc., 77% yield, 90% of exess to WWTP recovered
Ammonia	kg	6.70E-02	stoechiometric calc., 95% yield
Electricity, medium voltage	kWh	0.416	default estimation
heat, in chemical industry	MJ	2.35	default estimation
nitrogen	kg	0.019	default estimation
compressed air, 1000 kPa gauge	m3	0.5	default estimation
tap water	kg	2.60E-02	default estimation
Water, cooling, unspecified natural origin	m3	1.64E-02	default estimation
Water, river	m3	8.60E-04	default estimation
Water, well, in ground	m3	8.30E-04	default estimation
Chemical plant, organics	unit	4.00E-10	default estimation
Transport, by train	tkm	8.63E-01	standard distances & means
Transport, by lorry	tkm	1.44E-01	standard distances & means
OUTPUTS			
Ooleylamine	kg	1	
wastewater, average	m3	2.70E-06	default estimation
nitrogen, to air	kg	1.90E-02	default estimation
water, to air	m3	1.40E-03	default estimation
Oleic acid, to air	kg	2.74E-03	0.2% of input
Ammonia, to air	kg	1.34E-04	0.2% of input
carbon dioxide, fossil, to air	kg	7.89E-02	from waste water treatment
water, to water	m3	1.67E-02	default estimation
Oleic acid, to water	kg	3.13E-03	calculated from mass balances
Ammonium, to water	kg	9.65E-04	calculated from WWTP model
Nitrate, to water	kg	2.21E-03	calculated from WWTP model
COD, BOD	kg	1.48E-02	calculated from water emissions
TOC, DOC	kg	4.08E-03	calculated from water emissions

For the emission side, 0.2% of the starting materials (i.e. oleic acid and ammonia) are assumed to be emitted to air, the remaining part goes as part of the waste water flow into the waste water treatment plant (WWTP) like described in Hischier et al., 2005. 90% of this remaining oleic acid amount is recovered as oleic acid (… and thus deducted from the overall input amount here) while the remaining 10% goes into the WWTP process. Here, 90% are digested and transformed into carbon dioxide (emitted into air), while the remaining 10% pass the WWTP and thus are accounted as release into water. For ammonia, a removal efficiency for NH_4-N of 70% and for total N of 50% was assumed. The remaining emissions to water were considered as ammonium (NH_4) and nitrate (NO_3). The nitrogen emitted to air (N_2) and remaining in the sewage sludge was neglected. Table S.14 summarizes the resulting input and output values, used in this study to calculate the production efforts from 1 kg of oleylamine.

3.6. Manganese acetate

Anhydrous manganese(II) acetate ($Mn(CH_3COO)_2$, CAS No. 638-38-0) is a pale pink crystal solid at room temperature. It is soluble in water, methanol, acetic acid (Wikipedia Contributors, 2015). In the PhD thesis of Dai (Dai, 2014), the production pathway from manganese oxide (Mn_2O_3) – for which a respective dataset can be found in ecoinvent – to manganese(II) acetate, via the intermediates manganese sulphate and manganese carbonate, is reported in a simplified way. These reported datasets are used in this study.

3.7. Solvent recycling

In research institutions like e.g. University of Fribourg, all the liquid chemical waste is collected at the working places via collecting drums, distinguishing usually between halogenated organic solvents, halogen-free organic solvents as well as aqueous solutions of salts and heavy metals[1]. These drums are going to specialist companies for the further treatment of such waste. In his PhD thesis (Capello, 2006), Capello has analysed statistically the data of more than 100 waste solvent distillation processes in the chemical industry. In Capello et al., 2005, the resulting inventory data for this (average) waste solvent distillation process are reported – data that have been used here as model for the "default" situation of the treatment of waste solvent flows.

Table S.15 summarizes the various inputs and outputs of this recycling process.

Table S.15   Input and output data for the treatment of 1 kg of (used) solvents

[per kg solvent entering the recycling process]		Total	Remark
INPUTS			
Waste solvent, for treatement	kg	1	
Water, cooling, unspecified natural origin	m3	2.70E-02	Capello et al. 2005
Electricity, medium voltage	kWh	3.00E-02	Capello et al. 2005
Steam, in chemical industry	kg	1.40E+00	Capello et al. 2005
Nitrogen, liquid	kg	1.50E-03	Capello et al. 2005
transport, by lorry (7.5-16t)	tkm	2.00E-01	Capello et al. 2005
OUTPUTS			
recycled solvent	kg	7.10E-01	Capello et al. 2005
solvent, to hazardous waste incinerator	kg	2.90E-01	Capello et al. 2005
BENEFITS from hazardous waste treatment			
Electricity, high voltage	kWh	4.96E+00	calculated, based on default values in applied ecoinvent dataset (Doka, 2007)
Heat, from natural gas	MJ	1.84E-01	
Heat, from light fuel oil	MJ	1.84E-01	

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[1] Taken from „safety in the laboratory" presentation at http://www.chem.unifr.ch/assets/pdf/safety/security_course_e.pdf

4. RESULTS OF LCA-CALCULATIONS

4.1. Lab-Scale

Numerical LCA results for the production of 1 kg of cathode in case of the nano-structured $LiCoO_2$ (i.e. values shown in Figure 2 of the manuscript):

			LiCoO2	Composite	Electrode	Al-Foil
Fossil depletion	FDP	kg oil eq	1.61E+01	6.31E-01	1.55E+00	3.26E+00
Metal depletion	MDP	kg Fe eq	2.78E+00	3.46E-01	2.44E-01	3.02E-01
Climate Change	GWP	kg CO2 eq	5.69E+01	2.05E+00	1.16E+01	1.53E+01
Terrestrial acidification	TAP	kg SO2 eq	2.70E-01	7.27E-03	3.06E-02	1.22E-01
Freshwater eutrophication	FEP	kg P eq	2.69E-02	1.45E-03	3.93E-03	4.68E-03
Particulate matter formation	PMFP	kg PM10 eq	9.79E-02	3.01E-03	1.06E-02	4.33E-02
Photochemical oxidant formation	POFP	kg NMVOC	3.52E-01	5.01E-03	2.49E-02	5.92E-02
Human toxicity	HTP	kg 1,4-DB eq	2.76E+01	1.71E+00	2.10E+00	5.58E+00
Freshwater ecotoxicity	FETP	kg 1,4-DB eq	1.56E+00	2.66E-01	1.36E-01	2.00E-01
Marine ecotoxicity	METP	kg 1,4-DB eq	1.25E+00	2.34E-01	1.26E-01	1.92E-01

Numerical LCA results for the lab-scale production of 1 kg of LCO nanomaterial (i.e. values shown in Figure 3, upper part, of the manuscript):

	GWP	FDP	FETP	FEP	HTP	METP	MDP	PMFP	POFP	TAP
lithium methoxide	1.64E+01	4.82E+00	2.96E-01	1.10E-02	9.33E+00	2.82E-01	9.58E-01	4.26E-02	5.75E-02	1.02E-01
cobalt chloride	1.52E+01	3.49E+00	1.38E+00	4.51E-03	3.37E+01	1.49E+00	4.26E+00	8.32E-02	1.20E-01	1.20E-01
tetrahydrofurane	8.28E+00	3.11E+01	1.04E+00	2.24E-02	2.72E+01	9.06E-01	4.68E+00	1.66E-01	2.90E-01	5.03E-01
methanol	2.19E+00	2.61E+00	3.76E-02	4.10E-04	8.67E-01	1.98E-02	1.21E-01	6.02E-03	1.04E-02	2.40E-02
nitrogen	1.46E+02	4.13E+01	2.82E+00	1.09E-01	8.00E+01	2.63E+00	3.97E+00	1.94E-01	3.08E-01	5.87E-01
argon	8.52E+00	2.25E+00	1.01E-01	3.48E-03	2.81E+00	9.16E-02	1.36E-01	1.90E-02	2.51E-02	5.07E-02
water	4.34E-01	1.15E-01	1.77E-02	1.80E-04	2.33E-01	1.62E-02	3.65E-02	1.03E-03	1.42E-03	2.58E-03
electricity	1.27E+01	3.83E+00	1.70E+00	8.93E-03	1.08E+01	1.49E+00	2.22E+00	1.74E-02	2.83E-02	4.39E-02
solvent recycling	2.11E+01	-2.45E+00	1.05E+00	-1.43E-02	-1.62E+01	-2.04E-01	-1.37E+00	-8.40E-04	1.76E-02	2.59E-02
waste treatment	3.91E-01	3.66E-02	3.22E-03	1.30E-04	5.57E-02	3.09E-03	4.71E-03	3.00E-04	7.70E-04	8.50E-04
direct releases	1.44E+00	0.00E+00	9.85E-05	0.00E+00	4.52E-01	3.03E-03	0.00E+00	5.14E-06	1.04E+00	8.36E-08

Numerical LCA results for the lab-scale production of 1 kg of LMP nanomaterial (i.e. values shown in Figure 3, lower part, of the manuscript):

	GWP	FDP	FETP	FEP	HTP	METP	MDP	PMFP	POFP	TAP
lithium hydroxide	2.07E+00	5.24E-01	3.49E-02	1.27E-03	9.87E-01	3.31E-02	1.81E-01	4.47E-03	7.97E-03	1.24E-02
manganese acetate	4.90E+00	1.87E+00	9.01E-02	1.96E-03	2.29E+00	8.27E-02	4.78E+01	1.02E-02	1.82E-02	3.03E-02
phosphoric acid	7.49E-01	3.11E-01	3.12E-02	1.47E-03	7.12E-01	3.05E-02	1.21E-01	3.47E-03	4.11E-03	1.03E-02
benzyl ether	8.15E+01	3.89E+01	1.00E+00	2.12E-02	3.18E+01	1.01E+00	4.74E+00	1.31E-01	2.86E-01	3.56E-01
oleylamine	1.61E+01	1.77E+00	1.56E-01	2.99E-03	2.76E+00	1.13E-01	7.70E-01	2.39E-02	3.65E-02	4.68E-02
oleic acid	1.66E+00	1.25E-01	1.47E-02	2.90E-04	2.24E-01	9.43E-03	6.80E-02	2.43E-03	3.79E-03	4.28E-03
chloroform	5.95E+01	1.23E+01	5.55E-01	1.30E-02	1.18E+02	5.24E-01	2.36E+00	5.21E-02	8.91E-02	1.47E-01
hexane	6.27E+00	8.98E+00	8.60E-02	1.29E-03	2.00E+00	7.79E-02	5.48E-01	1.48E-02	8.32E-02	4.74E-02
electricity	1.84E+02	5.55E+01	2.47E+01	1.30E-01	1.56E+02	2.17E+01	3.22E+01	2.53E-01	4.11E-01	6.38E-01
solvent recycling	6.94E+01	-8.09E+00	3.45E+00	-4.72E-02	-5.34E+01	-6.71E-01	-4.51E+00	-2.76E-03	5.80E-02	8.53E-02
waste treatment	8.12E-02	7.61E-03	6.70E-04	2.76E-05	1.16E-02	6.40E-04	9.80E-04	6.13E-05	1.60E-04	1.80E-04
direct releases	0.00E+00	0.00E+00	3.04E-01	0.00E+00	1.10E-05	1.05E-05	0.00E+00	0.00E+00	2.04E-01	0.00E+00

4.2. (future) Pilot Production

Numerical LCA results for the (theoretical) pilot production of 1 kg of LCO nanomaterial (i.e. values shown in Figure 4, upper part, of the manuscript):

	FDP	MDP	GWP	TAP	FEP	PMFP	POFP	HTP	FETP	METP
lithium methoxide	4.38E+00	8.71E-01	1.49E+01	9.23E-02	9.96E-03	3.88E-02	5.23E-02	8.49E+00	2.69E-01	2.57E-01
cobalt chloride	3.30E+00	4.02E+00	1.44E+01	1.13E-01	4.26E-03	7.86E-02	1.14E-01	3.18E+01	1.31E+00	1.41E+00
solvents	2.39E-01	1.68E-02	2.99E-01	2.58E-03	6.79E-05	7.20E-04	1.25E-03	1.09E-01	4.48E-03	2.98E-03
inert gas	1.79E-01	1.72E-02	6.33E-01	2.54E-03	4.70E-04	8.40E-04	1.33E-03	3.46E-01	1.22E-02	1.14E-02
water	2.30E-02	7.31E-03	8.70E-02	5.20E-04	3.53E-05	2.10E-04	2.80E-04	4.67E-02	3.54E-03	3.24E-03
electricity	7.72E-01	4.47E-01	2.55E+00	8.87E-03	1.80E-03	3.51E-03	5.71E-03	2.17E+00	3.43E-01	3.02E-01
heat (natural gas)	9.94E-03	2.70E-04	2.93E-02	5.00E-05	1.25E-06	1.71E-05	6.17E-05	1.19E-03	4.29E-05	3.99E-05
waste treatment	6.61E-02	1.61E-02	6.79E-01	1.64E-03	2.78E-04	5.72E-04	1.42E-03	1.08E-01	6.76E-03	6.40E-03
direct emissions	0.00E+00	0.00E+00	1.35E+00	0.00E+00	3.25E-06	0.00E+00	7.17E-02	6.57E-02	5.31E-06	4.24E-05

Numerical LCA results for the (theoretical) pilot production of 1 kg of LMP nanomaterial (i.e. values shown in Figure 4, lower part, of the manuscript):

	FDP	MDP	GWP	TAP	FEP	PMFP	POFP	HTP	FETP	METP
lithium hydroxide	2.21E-01	7.66E-02	8.74E-01	5.23E-03	5.40E-04	1.90E-03	3.40E-03	4.19E-01	1.48E-02	1.41E-02
manganese acetate	1.97E+00	5.03E+01	5.16E+00	3.19E-02	2.07E-03	1.07E-02	1.91E-02	2.41E+00	9.48E-02	8.71E-02
phosphoric acid	4.34E-01	1.69E-01	1.04E+00	1.43E-02	2.05E-03	4.84E-03	5.73E-03	9.91E-01	4.34E-02	4.25E-02
solvents	5.35E-01	7.34E-02	1.43E+00	5.19E-03	3.30E-04	1.94E-03	4.31E-03	1.34E+00	1.57E-02	1.50E-02
electricity	2.18E-01	1.26E-01	7.21E-01	2.50E-03	5.10E-04	9.90E-04	1.61E-03	6.12E-01	9.69E-02	8.51E-02
heat (natural gas)	1.09E-01	3.06E-03	3.21E-01	5.50E-04	1.38E-05	1.80E-04	6.50E-04	1.32E-02	4.80E-04	4.40E-04
waste treatment	2.51E-02	3.23E-03	2.68E-01	5.80E-04	9.10E-05	2.00E-04	5.30E-04	3.82E-02	2.21E-03	2.12E-03
direct emissions	0.00E+00	3.32E-04	4.34E+00	5.37E-05	1.02E-02	0.00E+00	2.07E-01	4.78E+00	4.57E-04	7.53E-03

Numerical relative changes of the result of the (theoretical) pilot production of 1 kg of (LCO, LMP) nanomaterial when changing the various key elements from the lower to the higher value (i.e. values shown in Figure 5 of the manuscript):

		FDP	MDP	GWP	TAP	FEP	PMFP	POFP	HTP	FETP	METP
LCO	material input	3.43E-02	3.13E-02	3.73E-02	3.41E-02	3.29E-02	3.44E-02	2.63E-02	3.13E-02	3.11E-02	3.11E-02
	amount of inert gas	3.45E-03	7.83E-04	3.40E-03	2.49E-03	2.74E-03	1.52E-03	1.29E-03	1.15E-03	5.04E-04	4.91E-04
	losses of solvents	1.67E-02	4.10E-03	5.37E-03	6.69E-03	1.37E-03	4.21E-03	2.23E-01	1.88E-03	6.00E-04	4.23E-04
	electricity consumption	9.64E-02	1.67E-01	8.73E-02	4.12E-02	6.30E-02	3.30E-02	2.83E-02	5.23E-02	3.01E-02	2.89E-02
LMP	material input	4.67E-02	5.59E-02	5.58E-02	5.17E-02	2.32E-02	5.29E-02	1.22E-02	2.23E-02	5.20E-02	4.91E-02
	losses of solvents	2.34E-01	1.55E-03	3.05E-01	1.29E-01	3.23E-02	1.29E-01	8.08E-01	5.97E-01	1.12E-01	1.65E-01
	electricity consumption	5.93E-02	1.85E-03	6.30E-02	3.39E-02	3.91E-02	3.65E-02	7.39E-03	5.46E-02	1.68E-01	1.58E-01

Numerical relative results representing the range of the environmental impact of the (theoretical) pilot production processes for LCO and LMP relative tos the respective lab-scale impacts (set each time 100%) (i.e. values shown in Figure 6 of the manuscript):

	FDP	MDP	GWP	TAP	FEP	PMFP	POFP	HTP	FETP	METP
nano LCO, low	5.63E-02	1.41E-01	6.14E-02	8.07E-02	1.19E-01	1.03E-01	5.60E-02	1.83E-01	2.52E-01	2.86E-01
nano LCO, high	1.16E-01	3.04E-01	1.25E-01	1.57E-01	2.36E-01	1.99E-01	1.29E-01	3.58E-01	4.80E-01	5.45E-01
nano LMP, low	2.98E-02	7.22E-01	2.88E-02	5.17E-02	9.24E-02	5.08E-02	1.81E-01	4.92E-02	1.73E-02	2.63E-02
nano LMP, high	4.00E-02	7.65E-01	4.09E-02	6.27E-02	1.62E-01	6.19E-02	3.31E-01	8.24E-02	2.31E-02	3.60E-02

4.3. Comparison with other cathode materials

Numerical LCA results of the impacts for the production of 1 kg of various Li-containing cathode materials (i.e. values shown in Figure 7 of the manuscript):

	Unit	nano-LiCoO2	LiCoO2	Li-NMC	LiFePO4	LiMn2O4	nano-LiMnPO4
fossil depletion - FDP	kg oil-Eq	8.78E+00	5.62E+00	2.57E+00	1.72E+00	1.11E+00	3.97E+00
metal depletion - MDP	kg Fe-Eq	2.00E+00	1.24E+00	3.22E+01	4.73E-01	7.40E+01	5.07E+01
climate change - GWP100	kg CO2-Eq	3.21E+01	2.12E+01	1.06E+01	5.83E+00	4.32E+00	1.25E+01
terrestrial acidification - TAP100	kg SO2-Eq	1.89E-01	1.37E-01	3.98E-01	3.78E-02	1.81E-02	6.44E-02
freshwater eutrophication - FEP	kg P-Eq	3.94E-02	3.09E-02	1.74E-02	4.59E-03	2.21E-03	1.76E-02
particulate matter formation - PMFP	kg PM10-Eq	1.07E-01	7.77E-02	1.06E-01	1.56E-02	8.49E-03	2.74E-02
photochemical oxidant formation - POFP	kg NMVOC	2.13E-01	1.11E-01	8.05E-02	1.97E-02	1.09E-02	1.95E-01
human toxicity - HTPinf	kg 1,4-DCB-Eq	5.62E+01	4.72E+01	2.78E+01	3.39E+00	1.88E+00	1.52E+01
freshwater ecotoxicity - FETPinf	kg 1,4-DCB-Eq	4.10E+00	3.74E+00	1.05E+00	9.70E-02	5.37E-02	2.07E-01
marine ecotoxicity - METPinf	kg 1,4-DCB-Eq	3.95E+00	3.61E+00	1.02E+00	9.02E-02	4.98E-02	2.05E-01

Numerical LCA results of the impacts for 1 kWh of stored energy for the various Li-containing cathode materials (i.e. values shown in Figure 8, upper part, of the manuscript):

		nano-LCO	HT-LCO	Li-NMC	LFP	LMO	nano-LMP
fossil depletion - FDP	kg oil-Eq	2.42E-05	1.24E-05	2.82E-06	2.10E-06	5.03E-06	4.78E-06
metal depletion - MDP	kg Fe-Eq	5.51E-06	2.73E-06	3.53E-05	5.80E-07	3.37E-04	6.11E-05
climate change - GWP100	kg CO2-Eq	8.83E-05	4.68E-05	1.16E-05	7.15E-06	1.96E-05	1.50E-05
terrestrial acidification - TAP100	kg SO2-Eq	5.20E-07	3.03E-07	4.36E-07	4.63E-08	8.24E-08	7.75E-08
freshwater eutrophication - FEP	kg P-Eq	1.09E-07	6.80E-08	1.91E-08	5.62E-09	1.00E-08	2.12E-08
particulate matter formation - PMFP	kg PM10-Eq	2.95E-07	1.71E-07	1.16E-07	1.92E-08	3.86E-08	3.30E-08
photochemical oxidant formation - POFP	kg NMVOC	5.88E-07	2.44E-07	8.82E-08	2.41E-08	4.97E-08	2.34E-07
human toxicity - HTPinf	kg 1,4-DCB-Eq	1.55E-04	1.04E-04	3.05E-05	4.16E-06	8.53E-06	1.82E-05
freshwater ecotoxicity - FETPinf	kg 1,4-DCB-Eq	1.13E-05	8.24E-06	1.15E-06	1.19E-07	2.44E-07	2.50E-07
marine ecotoxicity - METPinf	kg 1,4-DCB-Eq	1.09E-05	7.96E-06	1.12E-06	1.11E-07	2.26E-07	2.46E-07

Numerical LCA results of the impacts for 1 Ah of available capacity for the various Li-containing cathode materials (i.e. values shown in Figure 8, lower part, of the manuscript):

		nano-LCO	HT-LCO	Li-NMC	LFP	LMO	nano-LMP
fossil depletion - FDP	kg oil-Eq	9.44E-08	5.35E-08	1.07E-08	7.15E-09	2.01E-08	1.96E-08
metal depletion - MDP	kg Fe-Eq	2.15E-08	1.18E-08	1.34E-07	1.97E-09	1.35E-06	2.51E-07
climate change - GWP100	kg CO2-Eq	3.45E-07	2.02E-07	4.43E-08	2.43E-08	7.85E-08	6.15E-08
terrestrial acidification - TAP100	kg SO2-Eq	2.03E-09	1.31E-09	1.66E-09	1.57E-10	3.30E-10	3.18E-10
freshwater eutrophication - FEP	kg P-Eq	4.24E-10	2.94E-10	7.27E-11	1.91E-11	4.01E-11	8.72E-11
particulate matter formation - PMFP	kg PM10-Eq	1.15E-09	7.40E-10	4.43E-10	6.51E-11	1.54E-10	1.35E-10
photochemical oxidant formation - POFP	kg NMVOC	2.30E-09	1.06E-09	3.35E-10	8.20E-11	1.99E-10	9.62E-10
human toxicity - HTPinf	kg 1,4-DCB-Eq	6.04E-07	4.50E-07	1.16E-07	1.41E-08	3.41E-08	7.48E-08
freshwater ecotoxicity - FETPinf	kg 1,4-DCB-Eq	4.41E-08	3.56E-08	4.36E-09	4.04E-10	9.77E-10	1.02E-09
marine ecotoxicity - METPinf	kg 1,4-DCB-Eq	4.25E-08	3.44E-08	4.25E-09	3.76E-10	9.05E-10	1.01E-09

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