SUPPLEMENTARY INFORMATION I (SI1)

On the environmental competitiveness of Sodium-Ion batteries under a full life cycle perspective – A cell-chemistry specific modelling approach

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This supplementary document contains additional information about the inventory modelling and the underlying calculation tool, and additional results tables and figures.

Two separate MS-Excel spreadsheets contain all numerical results including the data used for creating all graphs (SI 2), and the Excel-based dimensioning tool (SI 3)

The inventory data used for calculating the results are also provided as JSON-LD files for direct import into openLCA; and in ILCD format for import into other LCA software. The LCI is based on ecoinvent 3.7; use with other ecoinvent versions might require re-linking of flows.

All files are available for download on Zenodo:

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1. Battery modelling

The battery modelling is based on the BatPac tool developed by Argonne National Laboratories (ANL) (Nelson et al. 2019). However, being BatPac designed for sizing automotive batteries, it is little handy for dimensioning and evaluating individual cells, required for a prospective assessment of emerging batteries. The BatPac model has therefore been modified substantially, eliminating all components related with the battery pack, allowing to calculate battery composition based on performance targets on cell level. Electrochemical parameters for the assessed SIB have been introduced, and a recycling section was added that calculates the output of the different recycling processes in a parametrized way, automatically scaling inputs of process chemicals according to stoichiometric considerations and the individual cell composition. On the other hand, economic calculations have been eliminated to keep the tool simple and easy to adapt to future cell chemistries, giving it an environmental life cycle assessment scope. The tool also contains a sheet where the results are presented readily in tabulated inventory data format for the individual sub-processes, allowing easy introduction into LCA software.

Like the original BatPac tool, the calculation is iterative, and iterative calculation needs to be activated in the MS-Excel setup. Target capacity and target cell power are user input fields (orange), while electrochemical parameters are taken from the data collection sheet ("Chem"), but can be overridden by manual input in the light green fields. The Excel tool is provided for re-use and further update as separate file with the supplementary information.

1.1. Battery cell layout

The tool requires as input the target cell capacity and target battery power ("Battery Design", Lines 62 and 62), and calculates the cell size and performance according to the provided electrochemical parameters. As default, a 160 Wh prismatic cell is assumed, with target power of 800W (2C rate).

1.2. Cell performance

The cell performance parameters are obtained directly from the Excel calculation tool, with the corresponding energy densities and mass balances provided in Table 1 of the main manuscript. Electrochemical performance parameters are provided in the folder "Chem" within the XL calculator, and new cell chemistries with the corresponding electrochemical parameters can be introduced there.

1.3. Manufacturing energy demand

Due to the high share the cell manufacturing process contributes to the total potential environmental impacts of LIB production, the energy demand of cell manufacturing has been a field of intense scientific discussion, being data from cell manufacturers difficult to obtain and modelling approaches associated with high uncertainties (Peters et al. 2017; Peters and Weil 2018; Ellingsen et al. 2017). However, several recent works provided increasing evidence that the energy demand was overestimated initially (Emilsson and Dahllöf 2019; Dai et al. 2019). While the available data on manufacturing demand become more reliable, still little information is available about how these vary with different cell chemistries and energy densities. To overcome this limitation and obtain cell-specific energy demand values, we use energy demand according to the latest state of knowledge (provided for LiNMC cells) and scale these according to the specific cell properties. More specifically, we assume a total electricity demand of 32.5MJ per kWh of battery cell, of that 26MJ (75%) for the dry room and 6.5 MJ for other purposes, and 140MJ of heat, driven to 50% by the dry room and 50% by the electrode drying process (Dai et al. 2019), in line with other works (Yuan et al. 2017; Deng et al. 2017; Jinasena et al. 2021). These values are used for the NMC-type LIB (energy density 272Wh/kg), and then scaled according to the cell capacity and electrode area. The share of energy demand attributable to the dry room is scaled with energy density, assuming that energy demand scales with the size of the dry room and thus inversely with the energy density of the cells. The remaining energy demand, driven majorly by electrode drying and processing (Pettinger and Dong 2016) is scaled according to the calculated electrode area. The individual manufacturing energy demand obtained by that for each cell type is provided in Table S1 and can be modified directly in the Excel calculation tool.

Table S1. Energy demand for battery cell manufacturing (per cell)

	NaFCN	NaNMMT	NaMMO	NaMVP	NaNMC	NMC622	LFP	Unit
Electr. (dry room)	2.52	1.81	1.98	2.04	2.28	1.14	1.57	kWh
Electricity (other)	1.10	0.39	0.43	0.63	0.47	0.29	0.52	kWh
Heat (dry room)	24.47	17.56	19.19	19.80	22.12	11.09	15.24	MJ
Heat (other)	42.69	15.02	16.77	24.57	18.28	11.09	20.12	MJ

2. Material synthesis

The inventory data for the NaNMMT and NaNMC cell active materials are majorly taken from previous publications and updated to the latest ecoinvent version (3.7.1). This required substituting cobalt sulfate by cobalt carbonate, since $CoSO_4$ is no longer available in the database. These adaptations have been made based on stoichiometric calculations and are not described in detail. However, they are provided in the Excel calculation sheet for verification. Materials that have been modelled completely new are described in the following.

2.1. Sodium Magnesium Manganese Oxide (NaMMO)

The inventory data for the production of sodium magnesium manganese oxide, the cathode active material for the NaMMO SIB cells, is derived from the corresponding inventory for LIB, LiMO (Notter et al. 2010), which shows a similar structure and synthesis process. The input of lithium carbonate is substituted by sodium carbonate based on stoichiometric calculations, and the remaining inputs are adjusted to the different input flows. The corresponding tabulated inventory data is provided in the Excel calculation sheet.

2.2. Sodium Nickel Manganese Cobalt Oxide (NaNMC)

For the NaNMC and NaNMMT active materials, the inventory data is taken from previous publications (Mohr et al. 2020a; Peters et al. 2016), but also provided in the supplementary Excel sheet.

2.3. Prussian Blue (NaFNC)

The Prussian Blue active material (NaFNC) is obtained from sodium ferrocyanide and iron (III) chloride, with the stoichiometry adjusted to yield the desired sodium iron ferrocyanide ($Na_2Fe[Fe(CN)_6]$) (Yan et al. 2020). The sodium ferrocyanide precursor is synthesized from the reaction of hydrogen ferrocyanide, sodium hydroxide and iron(III) chloride.(Wiedeman et al. 1972) Heat and electricity demand are estimated for the main processing steps with the basic engineering toolbox (Engineering ToolBox 2019). The complete inventory data for the PBA synthesis process is provided in the supplementary Excel calculation sheet.

2.4. Sodium Manganese Vanadium Phosphate (NaMVP)

The polyanionic NaMVP active material is synthesised from Vanadium(III) acetylacetonate, Manganese acetate, Sodium acetate and phosphoric acid (molar ratio 1:1:4:3) in an ethanol solution at 60°C (Zhou et al. 2016). The precursor materials are obtained from the reaction of sodium carbonate and manganese carbonate with acetic acid, and of vanadium pentoxide with acetylacetone (Ullmann et al. 1995; Perry and Green 1999). The amounts of precursor are estimated assuming stoichiometric calculations with a gross excess input of 5%. Acetylacetone is prepared industrially by the thermal rearrangement of isopropenyl acetate (Ullmann et al. 1995), and, due to the lack of suitable inventory data in the ecoinvent database, the equivalent amount of propyl acetate is accounted for instead. The ethanol required as solvent is recovered internally, assuming a recovery of the active material at 50% water content and a loss (emissions to air) of 2% during the drying process (Althaus et al. 2007). CO_2 emissions to air (process emissions) are quantified based on the reaction stoichiometry (5mol CO_2/mol NaMVP), and accounting with standard air emission factors (0.2% of process chemicals) (Althaus et al. 2007). The unreacted (excess) chemicals constitute, together with the process water, a wastewater effluent that is sent to a treatment facility. Electricity and heat demand for the material synthesis and annealing process is taken from a previous publication for LiMO active materials (Notter et al. 2010), assuming that the process conditions do not vary substantially for different active materials. The complete inventory data for the process is provided in the supplementary Excel calculation sheet.

3. Material characteristics

The electrochemical characteristics (especially energy density) are of high importance for the calculation of the battery cell layout and the final mass balance and therefore their environmental impacts. These are derived from a literature review on SIB chemistries and their electrochemical properties, with those selected as basis for the cell dimensioning resumed in Table S2.

Table S2. Overview of the discussed sodium-ion cathode materials, their stoichiometry, structure, practical specific capacity, average potential vs. Na^+/Na, and specific energy; the specific energy is calculated for these cathode materials when combined with a sodium metal and hard carbon, respectively. For the hard carbon anode, a specific capacity of 240 mAh g^{-1} and an average potential of 0.2 V against Na^+/Na is assumed.

Acronym	Stoichiometry	Structure type	Practical specific capacity (mAh g^{-1})	Average potential (V vs. Na^+/Na)	Specific energy vs. Na (Wh kg^{-1})	Specific energy vs. hard carbon (Wh kg^{-}	Literature
NaNMMT	$Na_{1.1}(Ni_{0.3}Mn_{0.5}Mg_{0.05}Ti_{0.05})O_2$	layered oxide	150	3.20	425	277	(Peters et al. 2016)
NaMMO	$Na_{2/3}(Mn_{0.95}Mg_{0.05})O_2$	layered oxide	170	280	415	259	(Clément et al. 2016)
NaMVP	$Na_4MnV(PO_4)_3$	NASICON	101	3.45	321	231	(Zhou et al. 2016)
NaNMC	$Na_{1.05}(Ni_{0.33}Mn_{0.33}Co_{0.33})_{0.95}O_2$	layered oxide	120	2.80	305	208	(Sathiya et al. 2012)
NaPBA	$Na_2Fe[Fe(CN)_6]$	prussian blue analogue	120	2.90	316	216	(Ye et al. 2016),

4. Recycling processes

Though only the advanced hydrometallurgical process is modelled in detail and used for the present assessment, two other recycling processes are also provided in the Excel calculation tool. However, the underlying literature is considered insufficient for creating a reliable process model and bears the risk of substantially underestimating potential impacts from recycling due to the omission of relevant inputs and process steps in the modelling. The pyrometallurgical and the hydrometallurgical process as described in the following are therefore not recommended for direct use but can be improved and developed further for future assessments.

4.1. Pyrometallurgical recycling

A simple model based on literature data (Fisher et al. 2006), which is also the basis for the pyrometallurgical process provided by ecoinvent (Wernet et al. 2016). However, due to a substantial lack of data (the pyrometallurgical process obtains an alloy or matte containing the recovered metals, which needs to be processed further by hydrometallurgy for recovering the individual metals, what is not considered in the inventory) its use is not recommended. The inventory is provided nevertheless allowing future works to improve it.

4.2. Hydrometallurgical recycling

Also the hydrometallurgical process is modelled based on literature data (Fisher et al. 2006; Mohr et al. 2020a) and corresponds to the hydrometallurgical recycling process provided by ecoinvent. However, it also contains some major shortcomings. In particular, the overall energy demand and process inputs seems to be underestimated. We use the underlying inventory data and re-estimate the inputs of chemical products acc. to stoichiometric calculations (the exact calculation approach can be derived from the Excel tool), but still the process flow is very simple and the environmental impacts associated with the process itself (not the benefit from recovery) is likewise underestimated, which is why it is not further used in this work.

4.3. Advanced hydrometallurgical recycling:

The advanced hydrometallurgical process offers a deep recycling including recovery of anode active material and the electrolyte and is based on the process technology patented by Duesenfeld (Mohr et al. 2020b; Brückner et al. 2019). Material and energy inputs are estimated based on the underlying patents and various literature sources (Diekmann et al. 2017; Brückner et al. 2019; Mohr et al. 2020a), and the amount of process chemicals are then estimated based on stoichiometric calculations for every individual process step. This yields a complete and cell-specific inventory for every battery cell, provided completely in the Excel calculation tool. We therefore do not provide individual inventory tables for each cell chemistry within this document but refer to the Excel tool where these can be readily extracted.

5. Use-phase modellig

LIBs are already widely used in stationary applications starting from small home storage systems of some kWh of size (residential storage), medium size systems of multiple kWh (industrial applications) and large scale systems for ancillary services with capacities of multiple MWh (Figgener et al. 2020). The lifetime (calendric and cycles) of the battery systems, but also their round-trip efficiency have a high influence on the potential environmental impact from the use phase in stationary applications (Peters and Weil 2017; Vaalma et al. 2018; Le Varlet et al. 2020). Usually, the cycle life time is related to a retention capacity (RC) of 80 % which is often stated as the end of life of a lithium ion battery

(EOL). This cycle life time depends on several factors as temperature, c-rates and the depths of discharge (DoD) and can vary significantly depending on the testing conditions and the specific battery chemistry under investigation (Liu et al. 2019). Current state of the art LIBs can last for up to two decades for stationary storage (Harlow et al. 2019). Typical lifetimes for LFP are very high in comparison to other chemistries ranging from 2500 to more than 9000 equivalent full cycles with a depth of discharge rate of 80% and C-rates of 0.5 – 1 at 25°C until a retention rate of 80%. NMC is reported to deliver up to 2500 equivalent full cycles under the same conditions (Preger et al. 2020). However, also higher cycle numbers of up to over 4000 for equivalent full cycles have been reported for NMC pouch cells (Harlow et al. 2019).

For SIB, numbers in terms of cycle life vary e.g., from 50 cycles for a remaining capacity of 94.3% up to 20 000 cycles until a capacity of 54% for a similar type. Some reports more generically state that SIB achieve over 2000 full cycles (Bauer et al. 2018), while others specifically reported cycling capabilities of 4000 cycles with a DOD at 1 C for a capacity retention rate of 80% with a $Na_3V_2(PO_4)_2F_3$ cathode against hard carbon (Broux et al. 2019), which is compatible with current state of the art LIB technologies. There are start-up companies in the field of SIB such as Faradion indicating 1000 cycles for a retention rate of 70% (Faradion 2021), or Tiamat with over 5000 cycles at a remaining capacity of 80% using a not further specified polyanionic cathode material (Anon 2021). Of course, cycle lifetimes can be extended if a lower retention rate is accepted for stationary applications (e.g. lower than 70% instead of 80%), taking as example the secondary use of battery packs used before for mobility applications. Here degradation and capacity fade can be reduced by low c-rates and low DoD to extend battery life time (Kamath et al. 2020).

The round trip efficiency of SIBs is assumed to be comparable with those of LIB, reaching values of over 90% (Faradion 2021)(Peters et al. 2016) (Preger et al. 2020). Also, self-discharge rates for SiB are comparable to LiB. However, with a range of 1-2 % per month, this effect is negligible in case of daily operation. For other applications such as e.g., uninterrupted power supply with longer stand by times it might well be relevant.

For determining the amount of charge-discharge cycles within the assumed application, equivalent full cycles for battery operation with a DoD of 80% are used, with an energy to power ratio of 1 (i.e., the batter is discharged within one hour) (Baumann et al. 2017). Here, a representative use case is applied to conduct a sensitivity analysis and to benchmark the SIB against a state-of-the-art LiNMC and LiFP. The reference (functional unit) for this comparison is each converted kWh through the battery system required to provide a distinct service. The internal losses are attributed to the battery system, which can have a significant influence on their overall environmental impacts over their lifetime. Furthermore, the retention rate of 80 % is included to the initial sizing of the battery, to account for lower retention rates in later operation years. Two different electricity sources are considered: (i) photovoltaic (PV)-based and (ii) grid electricity mix for Europe. A fixed energy-to-power (E/P) ratio is considered for all systems and a total project lifetime of 20 years. Herein, the cells have to be exchanged in case of insufficient cycle or calendric life time. Additionally, a maximum Depth of Discharge of 80 % is assumed to maintain a reserve to increase battery lifetime. This corresponds to 1,460 operation hours per year. It has to be mentioned that the yearly operation time varies significantly based on the provided energy storage service and has a high impact on final results, which is why the results for the use phase are valid only for the assessed application case and cannot be generalized (Abbas A. Akhil, Georgianne Huff, Aileen B. Currier, Benjamin C. Kaun, Dan M. Rastler, and Stella Bingqing Chen, Andrew L. Cotter, Dale T. Bradshaw, and William D. Gauntlett 2013).

The impact of balance of plant (inverter, BMS, gears and switches) is assumed to be comparable for both LIB and SIB systems and is neglected in this assessment. This is in-line with the scope of the assessment that compares batteries on cell level, disregarding additional peripherical components.

However, different volumetric energy densities can lead to varying need of packaging materials, which could cause differences between the assessed cell chemistries. Also, different needs in terms of control electronics due to different fire or overheating risks might a subject of future assessments. The calendric lifetime does only play a role in case of applications with very low cycle numbers but has no relevance for the present application case. The key parameters regarding the use-phase of the battery cells are resumed in Table S3.

Table S3. Overview of use phase parameters calculated for the different battery types

	NaNMC	NaMVP	NaMMO	NaNMMT	NaPBA	LiNMC[622]	LiFP
Total cap kWh	3,152.17	3,118.28	3,152.17	3,152.17	3,118.28	3,152.17	3,118.28
Ex. Cell cycle	2.65	1.43	2.65	2.65	1.43	2.65	1.09
Ex Cell calendr.	1	1	1	1	1	1	1
Ex. Rate used	2.7	1.4	2.7	2.7	1.4	2.7	1.1
Total consumed Energy in kWh	2539130	2197849	2539130	2539130	2197849	2539130	2197849

6. Results

6.1. Numeric results for use phase

Figures S1 and S2 contain the results of the entire life cycle for electricity from PV and grid as well as with (S1) and without recycling (S2).

	Electricity from PV							Electricity from Grid						
AP	NaNMC	NaMVP	NaMMO	NaNMMT	NaPBA	LiNMC	LiFP	NaNMC	NaMVP	NaMMO	NaNMMT	NaPBA	LiNMC	LiFP
Production	0.040	0.068	0.022	0.021	0.031	0.016	0.023	0.040	0.068	0.022	0.021	0.031	0.016	0.023
Use	0.050	0.043	0.050	0.050	0.043	0.050	0.043	0.193	0.167	0.193	0.193	0.167	0.193	0.167
Replacemei	0.107	0.074	0.059	0.056	0.034	0.043	0.025	0.107	0.074	0.059	0.056	0.034	0.043	0.025
Total	0.196	0.186	0.131	0.126	0.108	0.109	0.092	0.340	0.310	0.275	0.269	0.232	0.252	0.216
W+	0.440	0.856	0.244	0.229	0.390	0.178	0.293	0.440	0.856	0.244	0.229	0.390	0.178	0.088
W-	0.040	0.031	0.036	0.036	0.028	0.035	0.027	0.124	0.098	0.124	0.124	0.098	0.124	0.098
GWP	NaNMC	NaMVP	NaMMO	NaNMMT	NaPBA	LiNMC	LiFP	NaNMC	NaMVP	NaMMO	NaNMMT	NaPBA	LiNMC	LiFP
Production	0.006	0.009	0.005	0.004	0.008	0.003	0.005	0.006	0.009	0.005	0.004	0.008	0.003	0.005
Use	0.008	0.007	0.008	0.008	0.007	0.008	0.007	0.037	0.032	0.037	0.037	0.032	0.037	0.032
Replacemei	0.016	0.009	0.013	0.011	0.009	0.008	0.005	0.016	0.009	0.013	0.011	0.009	0.008	0.005
Total	0.030	0.025	0.026	0.023	0.024	0.019	0.017	0.059	0.051	0.056	0.052	0.049	0.048	0.042
W+	0.065	0.109	0.054	0.044	0.099	0.032	0.058	0.065	0.161	0.095	0.093	0.099	0.080	0.075
W-	0.010	0.005	0.008	0.007	0.005	0.006	0.005	0.024	0.019	0.024	0.024	0.019	0.024	0.019
mHtox per l	NaNMC	NaMVP	NaMMO	NaNMMT	NaPBA	LiNMC	LiFP	NaNMC	NaMVP	NaMMO	NaNMMT	NaPBA	LiNMC	LiFP
Production	0.004	0.018	0.002	0.002	0.002	0.002	0.003	0.004	0.018	0.002	0.002	0.002	0.002	0.003
Use	0.008	0.007	0.008	0.008	0.007	0.008	0.007	0.015	0.013	0.015	0.015	0.013	0.015	0.013
Replacemei	0.010	0.020	0.004	0.004	0.002	0.005	0.003	0.010	0.020	0.004	0.004	0.002	0.005	0.003
Total	0.023	0.045	0.014	0.014	0.011	0.016	0.013	0.030	0.051	0.021	0.021	0.017	0.023	0.019
W+	0.043	0.227	0.017	0.017	0.026	0.023	0.035	0.043	0.227	0.017	0.017	0.026	0.023	0.011
W-	0.006	0.006	0.006	0.006	0.004	0.006	0.004	0.010	0.008	0.010	0.010	0.008	0.010	0.008
RDP per kW	NaNMC	NaMVP	NaMMO	NaNMMT	NaPBA	LiNMC	LiFP	NaNMC	NaMVP	NaMMO	NaNMMT	NaPBA	LiNMC	LiFP
Production	0.001	0.000	0.000	0.000	0.000	0.000	0.001	0.001	0.000	0.000	0.000	0.000	0.000	0.001
Use	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Replacemei	0.002	0.000	0.000	0.001	0.000	0.000	0.001	0.002	0.000	0.000	0.001	0.000	0.000	0.001
Total	0.004	0.002	0.002	0.002	0.002	0.002	0.002	0.003	0.001	0.001	0.001	0.001	0.001	0.002
W+	0.009	0.005	0.002	0.004	0.003	0.002	0.008	0.009	0.005	0.002	0.004	0.003	0.002	0.002
W-	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.000	0.000	0.001	0.000	0.000	0.000

Figure S1. Screenshot of numeric values for the use phase with recycling including electricity from PV (left tables) and from the public grid (right tables). W+ and W- represent min and max values. Numerical values are provided in a separate ESI document in Excel format.

	Electricity from PV							Electricity from Grid						
AP	NaNMC	NaMVP	NaMMO	NaNMMT	NaPBA	LiNMC622	LiFP	NaNMC	NaMVP	NaMMO	NaNMMT	NaPBA	LiNMC622	LiFP
Constr.	0.107	0.091	0.054	0.057	0.061	0.049	0.036	0.107	0.091	0.054	0.057	0.061	0.049	0.036
El. Cons	0.050	0.043	0.050	0.050	0.043	0.050	0.043	0.193	0.167	0.193	0.193	0.167	0.193	0.167
Batt exchar	0.283	0.099	0.143	0.152	0.066	0.129	0.039	0.283	0.099	0.143	0.152	0.066	0.129	0.039
Total	0.440	0.233	0.246	0.258	0.171	0.227	0.118	0.583	0.358	0.389	0.402	0.295	0.371	0.242
W+	1.171	1.143	0.589	0.626	0.766	0.533	0.448	1.171	1.143	0.589	0.626	0.766	0.533	0.135
W-	0.078	0.033	0.042	0.043	0.031	0.041	0.028	0.176	0.098	0.124	0.124	0.098	0.124	0.098
GWP	NaNMC	NaMVP	NaMMO	NaNMMT	NaPBA	LiNMC622	LiFP	NaNMC	NaMVP	NaMMO	NaNMMT	NaPBA	LiNMC622	LiFP
Constr.	0.009	0.010	0.006	0.005	0.009	0.005	0.005	0.009	0.010	0.006	0.005	0.009	0.005	0.005
El. Cons	0.008	0.007	0.008	0.008	0.007	0.008	0.007	0.037	0.032	0.037	0.037	0.032	0.037	0.032
Batt exchar	0.025	0.010	0.015	0.014	0.010	0.013	0.006	0.025	0.010	0.015	0.014	0.010	0.013	0.006
Total	0.042	0.027	0.029	0.028	0.027	0.026	0.018	0.072	0.052	0.058	0.057	0.052	0.055	0.043
W+	0.345	0.173	0.175	0.187	0.116	0.160	0.071	0.102	0.207	0.207	0.220	0.145	0.191	0.100
W-	0.007	0.005	0.006	0.006	0.005	0.006	0.005	0.024	0.019	0.024	0.024	0.019	0.024	0.019
mHtox per l	NaNMC	NaMVP	NaMMO	NaNMMT	NaPBA	LiNMC622	LiFP	NaNMC	NaMVP	NaMMO	NaNMMT	NaPBA	LiNMC622	LiFP
Constr.	0.013	0.019	0.002	0.003	0.003	0.011	0.011	0.013	0.019	0.002	0.003	0.003	0.011	0.011
El. Cons	0.008	0.007	0.008	0.008	0.007	0.008	0.007	0.015	0.013	0.015	0.015	0.013	0.015	0.013
Batt exchar	0.033	0.020	0.005	0.008	0.003	0.030	0.012	0.033	0.020	0.005	0.008	0.003	0.030	0.012
Total	0.054	0.046	0.015	0.020	0.013	0.049	0.029	0.061	0.052	0.022	0.027	0.019	0.056	0.035
W+	0.137	0.233	0.021	0.035	0.036	0.123	0.133	0.137	0.233	0.021	0.035	0.036	0.123	0.040
W-	0.009	0.006	0.006	0.006	0.004	0.008	0.005	0.021	0.008	0.010	0.010	0.008	0.019	0.008
RDP per kW	NaNMC	NaMVP	NaMMO	NaNMMT	NaPBA	LiNMC622	LiFP	NaNMC	NaMVP	NaMMO	NaNMMT	NaPBA	LiNMC622	LiFP
Constr.	0.004	0.001	0.001	0.001	0.001	0.003	0.003	0.004	0.001	0.001	0.001	0.001	0.003	0.003
El. Cons	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Batt exchar	0.010	0.001	0.002	0.003	0.001	0.009	0.004	0.010	0.001	0.002	0.003	0.001	0.009	0.004
Total	0.016	0.003	0.003	0.005	0.003	0.014	0.008	0.015	0.002	0.002	0.004	0.002	0.013	0.007
W+	0.043	0.010	0.006	0.011	0.011	0.038	0.041	0.043	0.010	0.006	0.011	0.011	0.038	0.012
W-	0.003	0.001	0.001	0.001	0.001	0.003	0.001	0.006	0.000	0.001	0.002	0.000	0.006	0.000

Figure S2. Screenshot of numeric values for the use phase without recycling including electricity from PV (left tables) and from the public grid (right tables). W+ and W- represent min and max values. Numerical values are provided in a separate ESI document in Excel format.

6.2. Sensitivity analysis, heat maps with grid electricity

Figures S1 and S2 contain the results (heat maps) of the sensitivity analysis for varying cycle life and round-trip efficiency when using grid electricity for charging.

Effi-ciency	NaNMC	NaMVP	NaMMO	NaNMMT	NaPBA	LiNMC	LiFP	NaNMC	NaMVP	NaMMO	NaNMMT	NaPBA	LiNMC	LiFP
Eff.	GWP gCO2 eq /kWh							ADP mgSb eq./kWh						
90%	69.943	66.609	66.416	62.897	64.907	58.934	57.797	0.0036	0.0013	0.0009	0.0016	0.0009	0.0010	0.0017
91%	64.438	61.140	60.950	57.470	59.458	53.550	52.426	0.0035	0.0012	0.0009	0.0015	0.0008	0.0010	0.0016
92%	59.053	55.791	55.603	52.160	54.127	**48.283**	47.171	0.0034	0.0012	0.0009	0.0015	0.0008	**0.0010**	0.0016
93%	53.784	50.557	50.370	46.965	48.910	43.129	**42.029**	0.0033	0.0011	0.0008	0.0014	0.0007	0.0009	0.0015
94%	48.626	45.433	45.249	41.880	43.805	38.085	36.997	0.0033	0.0011	0.0008	0.0014	0.0007	0.0009	0.0015
95%	43.577	40.418	40.236	36.902	38.806	33.147	32.071	0.0032	0.0010	0.0007	0.0013	0.0006	0.0008	0.0014
96%	38.634	35.508	35.327	32.028	33.913	28.312	27.247	0.0031	0.0010	0.0007	0.0013	0.0006	0.0008	0.0014
97%	33.792	30.698	30.519	27.255	29.120	23.577	22.523	0.0031	0.0009	0.0006	0.0012	0.0006	0.0007	0.0013
	AP mmolc H+ eq /kWh							HTP mCTUh/kWh						
90%	0.397	0.394	0.330	0.325	0.314	0.307	0.297	0.034	0.059	0.025	0.025	0.024	0.027	0.025
91%	0.368	0.365	0.302	0.297	0.286	0.280	0.269	0.032	0.056	0.023	0.023	0.022	0.025	0.023
92%	0.340	0.337	0.275	0.269	0.259	**0.252**	0.242	0.030	0.053	0.021	0.021	0.020	**0.023**	**0.021**
93%	0.312	0.310	0.248	0.243	0.232	0.226	**0.216**	0.027	0.051	0.019	0.019	0.017	0.021	0.019
94%	0.285	0.283	0.221	0.217	0.206	0.200	0.190	0.025	0.049	0.017	0.017	0.015	0.018	0.017
95%	0.259	0.256	0.196	0.191	0.180	0.174	0.165	0.023	0.046	0.015	0.015	0.013	0.016	0.015
96%	0.233	0.231	0.171	0.166	0.155	0.149	0.140	0.021	0.044	0.013	0.013	0.011	0.014	0.013
97%	0.208	0.205	0.146	0.141	0.131	0.125	0.115	0.019	0.042	0.011	0.011	0.010	0.013	0.011

Figure S3. Cradle-to-grave impacts per kWh of electricity provided by the battery cells over the lifetime of the assumed application with charge-discharge efficiency; charging electricity from grid. Numerical values are provided in a separate ESI document in Excel format.

Cycle life	NaNMC	NaMVP	NaMMO	NaNMMT	NaPBA	LiNMC	LiFP	NaNMC	NaMVP	NaMMO	NaNMMT	NaPBA	LiNMC	LiFP
Cycles	GWP gCO2 eq /kWh							ADP mgSb eq./kWh						
1000	123.78	159.25	109.97	96.20	147.72	80.69	99.56	0.0128	0.0063	0.0026	0.0050	0.0036	0.0030	0.0093
1500	95.01	116.98	85.81	76.63	109.29	66.29	77.18	0.0086	0.0043	0.0018	0.0034	0.0025	0.0021	0.0063
2000	80.63	95.84	73.73	66.84	90.08	59.09	66.00	0.0066	0.0033	0.0014	0.0026	0.0019	0.0016	0.0048
2500	72.00	83.16	66.48	60.97	78.55	54.77	59.29	0.0053	0.0027	0.0012	0.0022	0.0016	0.0014	0.0039
3000	66.24	74.71	61.64	57.05	70.87	51.88	54.81	0.0045	0.0023	0.0010	0.0018	0.0014	0.0012	0.0033
3500	62.14	68.67	58.19	54.26	65.38	49.83	51.62	0.0039	0.0020	0.0009	0.0016	0.0012	0.0010	0.0028
4000	59.05	64.14	55.60	52.16	61.26	**48.28**	49.22	0.0034	0.0018	0.0009	0.0015	0.0011	**0.0010**	0.0025
4500	56.66	60.62	53.59	50.53	58.06	47.08	47.36	0.0031	0.0016	0.0008	0.0013	0.0010	0.0009	0.0023
5000	54.74	57.80	51.98	49.22	55.50	46.12	45.86	0.0028	0.0015	0.0007	0.0012	0.0009	0.0008	0.0021
5500	53.17	55.50	50.66	48.16	53.40	45.34	44.64	0.0026	0.0014	0.0007	0.0011	0.0008	0.0008	0.0019
6000	51.86	53.58	49.56	47.27	51.65	44.68	43.63	0.0024	0.0013	0.0007	0.0011	0.0008	0.0007	0.0018
6500	50.76	51.95	48.63	46.51	50.18	44.13	42.77	0.0022	0.0012	0.0006	0.0010	0.0008	0.0007	0.0016
7000	49.81	50.56	47.84	45.87	48.91	43.65	42.03	0.0021	0.0011	0.0006	0.0010	0.0007	0.0007	0.0015
7500	49.30	49.81	47.41	45.52	48.23	43.40	41.64	0.0020	0.0011	0.0006	0.0009	0.0007	0.0007	0.0015
8000	49.30	49.81	47.41	45.52	48.23	43.40	41.64	0.0020	0.0011	0.0006	0.0009	0.0007	0.0007	0.0015
8500	49.30	49.81	47.41	45.52	48.23	43.40	41.64	0.0020	0.0011	0.0006	0.0009	0.0007	0.0007	0.0015
9000	49.30	49.81	47.41	45.52	48.23	43.40	41.64	0.0020	0.0011	0.0006	0.0009	0.0007	0.0007	0.0015
9500	49.30	49.81	47.41	45.52	48.23	43.40	41.64	0.0020	0.0011	0.0006	0.0009	0.0007	0.0007	0.0015
10000	49.30	49.81	47.41	45.52	48.23	43.40	41.64	0.0020	0.0011	0.0006	0.0009	0.0007	0.0007	0.0015
	AP mmolc H+ eq /kWh							HTP mCTUh/kWh						
1000	0.780	1.165	0.519	0.499	0.622	0.430	0.509	0.073	0.278	0.038	0.038	0.043	0.045	0.054
1500	0.584	0.833	0.410	0.397	0.470	0.351	0.395	0.053	0.190	0.030	0.030	0.033	0.035	0.040
2000	0.487	0.666	0.356	0.346	0.394	0.312	0.338	0.044	0.146	0.026	0.026	0.028	0.030	0.034
2500	0.428	0.566	0.323	0.315	0.349	0.288	0.304	0.038	0.119	0.024	0.024	0.025	0.027	0.029
3000	0.389	0.500	0.302	0.295	0.319	0.272	0.281	0.034	0.101	0.023	0.023	0.023	0.025	0.027
3500	0.361	0.452	0.286	0.280	0.297	0.261	0.265	0.032	0.089	0.022	0.022	0.022	0.024	0.025
4000	0.340	0.417	0.275	0.269	0.281	**0.252**	0.253	0.030	0.079	0.021	0.021	0.021	**0.023**	0.023
4500	0.323	0.389	0.265	0.261	0.268	0.246	0.243	0.028	0.072	0.020	0.020	0.020	0.022	0.022
5000	0.310	0.367	0.258	0.254	0.258	0.240	0.235	0.027	0.066	0.020	0.020	0.019	0.021	0.021
5500	0.300	0.349	0.252	0.249	0.250	0.236	0.229	0.026	0.061	0.019	0.019	0.019	0.021	0.021
6000	0.291	0.333	0.247	0.244	0.243	0.233	0.224	0.025	0.057	0.019	0.019	0.018	0.020	0.020
6500	0.283	0.321	0.243	0.240	0.237	0.230	0.220	0.024	0.054	0.019	0.019	0.018	0.020	0.019
7000	0.277	0.310	0.240	0.237	0.232	0.227	0.216	0.023	0.051	0.018	0.018	0.017	0.019	0.019
7500	0.273	0.304	0.238	0.235	0.229	0.226	0.214	0.023	0.049	0.018	0.018	0.017	0.019	0.019
8000	0.273	0.304	0.238	0.235	0.229	0.226	0.214	0.023	0.049	0.018	0.018	0.017	0.019	0.019
8500	0.273	0.304	0.238	0.235	0.229	0.226	0.214	0.023	0.049	0.018	0.018	0.017	0.019	0.019
9000	0.273	0.304	0.238	0.235	0.229	0.226	0.214	0.023	0.049	0.018	0.018	0.017	0.019	0.019
9500	0.273	0.304	0.238	0.235	0.229	0.226	0.214	0.023	0.049	0.018	0.018	0.017	0.019	0.019
10000	0.273	0.304	0.238	0.235	0.229	0.226	0.214	0.023	0.049	0.018	0.018	0.017	0.019	0.019

Figure S4. Cradle-to-grave impacts per kWh of electricity provided by the battery cells over the lifetime of the assumed application with varying cycle life; charging electricity from grid. Numerical values are provided in a separate ESI document in Excel format.

En. Dens. Wh/kg	GWP kgCO2 eq /kWh							ADP gSb eq./kWh						
	NaNMC	NaMVP	NaMMO	NaNMMT	NaPBA	**LiNMC**	LiFP	NaNMC	NaMVP	NaMMO	NaNMMT	NaPBA	**LiNMC**	LiFP
100	74.6	124.0	72.3	64.1	91.8	74.6	85.0	10.85	5.96	2.28	5.10	2.65	4.64	11.50
110	67.8	112.7	65.7	58.2	83.4	67.8	77.3	9.86	5.42	2.07	4.64	2.41	4.21	10.45
120	62.2	103.3	60.2	53.4	76.5	62.2	70.8	9.04	4.97	1.90	4.25	2.21	3.86	9.58
130	57.4	95.4	55.6	49.3	70.6	57.4	65.4	8.34	4.59	1.76	3.92	2.04	3.57	8.84
140	53.3	88.6	51.6	45.8	65.5	53.3	60.7	7.75	4.26	1.63	3.64	1.89	3.31	8.21
150	49.8	82.7	48.2	42.7	61.2	49.7	56.7	7.23	3.98	1.52	3.40	1.76	3.09	7.66
160	46.6	77.5	45.2	40.0	57.3	46.6	53.1	6.78	3.73	1.43	3.19	1.65	2.90	7.18
170	43.9	72.9	42.5	37.7	54.0	43.9	50.0	6.38	3.51	1.34	3.00	1.56	2.73	6.76
180	41.5	68.9	40.1	35.6	51.0	41.5	47.2	6.03	3.31	1.27	2.83	1.47	2.58	6.39
190	39.3	65.3	38.0	33.7	48.3	39.3	44.7	5.71	3.14	1.20	2.68	1.39	2.44	6.05
200	37.3	62.0	36.1	32.0	45.9	37.3	42.5	5.42	2.98	1.14	2.55	1.32	2.32	5.75
210	35.5	59.0	34.4	30.5	43.7	35.5	40.5	5.17	2.84	1.09	2.43	1.26	2.21	5.47
220	33.9	56.4	32.8	29.1	41.7	33.9	38.6	4.93	2.71	1.04	2.32	1.20	2.11	5.23
230	32.4	53.9	31.4	27.8	39.9	32.4	36.9	4.72	2.59	0.99	2.22	1.15	2.02	5.00
240	31.1	51.7	30.1	26.7	38.2	31.1	35.4	4.52	2.49	0.95	2.12	1.10	1.93	4.79
250	29.9	49.6	28.9	25.6	36.7	29.8	34.0	4.34	2.39	0.91	2.04	1.06	1.85	4.60
260	28.7	47.7	27.8	24.6	35.3	28.7	32.7	4.17	2.29	0.88	1.96	1.02	1.78	4.42
270	27.6	45.9	26.8	23.7	34.0	**27.6**	31.5	4.02	2.21	0.85	1.89	0.98	**1.72**	4.26
280	26.7	44.3	25.8	22.9	32.8	26.6	30.4	3.87	2.13	0.82	1.82	0.95	1.66	4.11

Wh/kg	AP mmolc H+ eq /kWh							HTP mCTUh/kWh						
	NaNMC	NaMVP	NaMMO	NaNMMT	NaPBA	**LiNMC**	LiFP	NaNMC	NaMVP	NaMMO	NaNMMT	NaPBA	**LiNMC**	LiFP
100	507.6	976.2	324.9	333.5	361.9	409.5	432.7	49.7	259.3	22.6	24.5	24.0	51.9	51.7
110	461.5	887.5	295.4	303.2	329.0	372.3	393.4	45.2	235.7	20.6	22.3	21.8	47.2	47.0
120	423.0	813.5	270.7	277.9	301.6	341.3	360.6	41.5	216.0	18.8	20.4	20.0	43.3	43.1
130	390.5	751.0	249.9	256.6	278.4	315.0	332.9	38.3	199.4	17.4	18.8	**18.5**	39.9	39.8
140	362.6	697.3	232.1	238.2	258.5	292.5	309.1	35.5	185.2	16.1	17.5	17.2	37.1	36.9
150	338.4	650.8	216.6	222.4	241.3	273.0	288.5	33.2	172.8	15.1	16.3	16.0	34.6	34.5
160	317.3	610.1	203.1	208.5	226.2	256.0	270.4	31.1	162.0	14.1	15.3	15.0	32.4	32.3
170	298.6	574.3	191.1	196.2	212.9	240.9	254.5	29.3	152.5	13.3	14.4	14.1	30.5	30.4
180	282.0	542.4	180.5	185.3	201.0	227.5	240.4	27.6	144.0	12.6	13.6	13.4	28.8	28.7
190	267.2	513.8	171.0	175.5	190.5	215.5	227.7	26.2	136.4	11.9	12.9	12.6	27.3	27.2
200	253.8	488.1	162.4	166.8	180.9	204.8	216.4	24.9	129.6	11.3	12.2	12.0	26.0	25.9
210	241.7	464.9	154.7	158.8	172.3	195.0	206.1	23.7	123.5	10.8	11.7	11.4	24.7	24.6
220	230.7	443.7	147.7	151.6	164.5	186.2	196.7	22.6	117.8	10.3	11.1	10.9	23.6	23.5
230	220.7	424.5	141.3	145.0	157.3	178.1	188.1	21.6	112.7	9.8	10.7	10.4	22.6	22.5
240	211.5	406.8	135.4	139.0	150.8	170.6	180.3	20.7	108.0	9.4	10.2	10.0	21.6	21.5
250	203.1	390.5	130.0	133.4	144.8	163.8	173.1	19.9	103.7	9.0	9.8	9.6	20.8	20.7
260	195.2	375.5	125.0	128.3	139.2	157.5	166.4	19.1	99.7	8.7	9.4	9.2	20.0	19.9
270	188.0	361.6	120.3	123.5	134.0	**151.7**	160.3	18.4	96.0	8.4	9.1	8.9	**19.2**	19.2
280	181.3	348.7	116.0	119.1	129.2	146.3	154.5	17.8	92.6	8.1	8.7	8.6	18.5	18.5

Figure S5. Cradle-to-grave impacts per kWh of electricity provided by the battery cells over the lifetime of the assumed application with varying cell energy density; charging electricity from grid. Numerical values are provided in a separate ESI document in Excel format.

6.3. Sensitivity analysis, graphs with varying energy density

Figure S6 shows the net impacts (production minus recycling benefit; without use-phase) of the battery cells with varying energy density (variation relative to the base case assumption for each cell type).

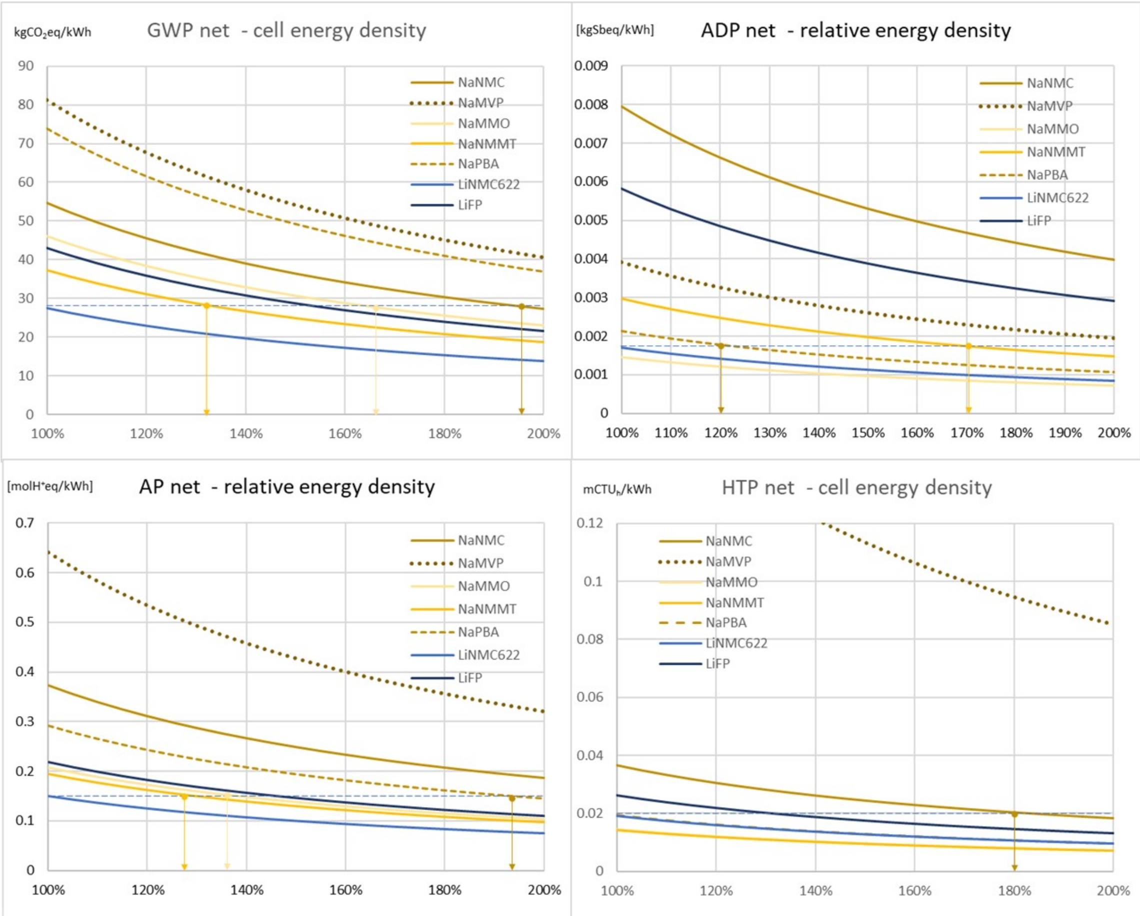

Figure S6 Net impacts (production minus recycling benefits) with varying energy density. The vertical arrows mark break-even points when other cell chemistries equal the results of the LiNMC cell. The underlying values are provided in a separate ESI document in Excel format.

6.4. Sensitivity analysis, graphs with varying recycling rate

Figure S3 provides the net impacts (production minus recycling benefit; without use-phase) for the assessed cells when assuming varying recycling quota. Recycling quota refers to the share of cells that are actually EoL treated (recycled). Note that this is a hypothetical consideration, and that different assessment scopes are mixed (for the cells where no recycling is accounted for, only the production impacts are used, and no alternative EoL handling like e.g., incineration is modelled). The results are therefore valid only for visualizing the sensitivity of the results on the recycling quota.

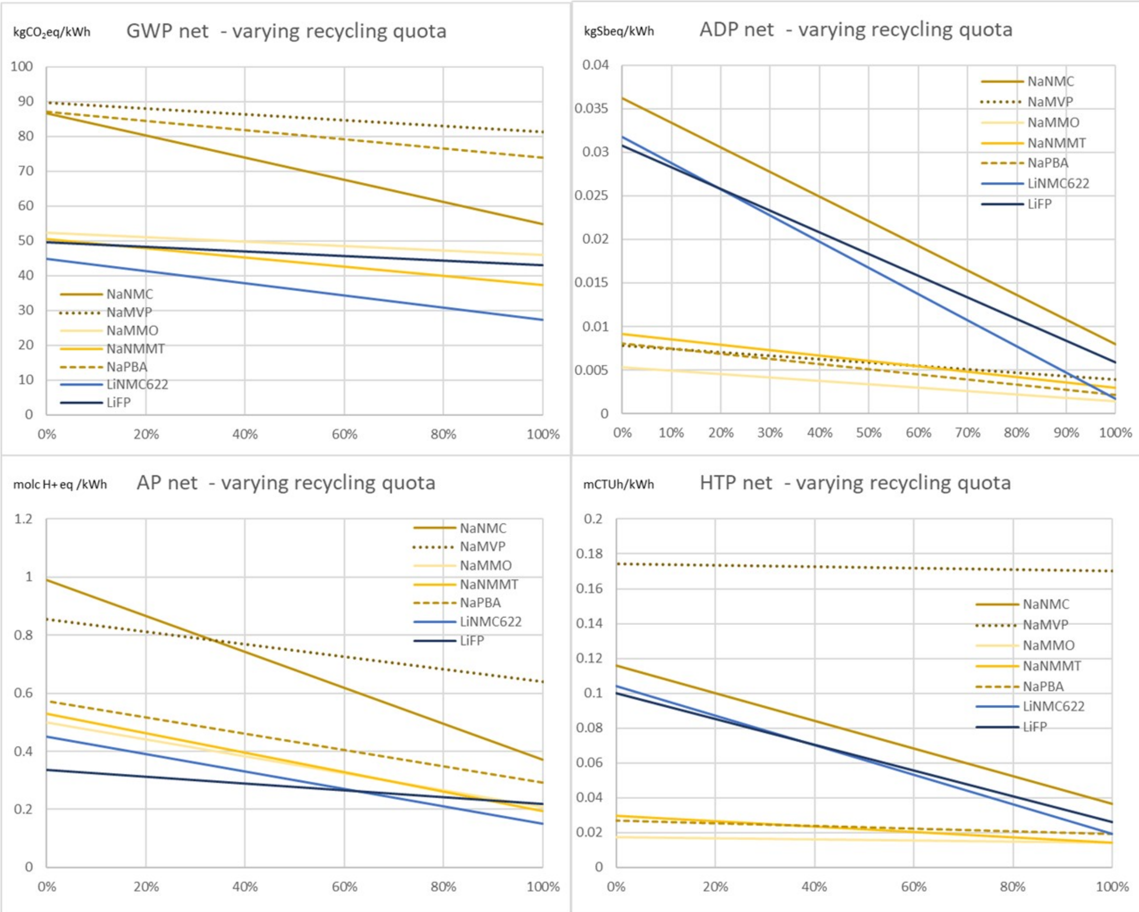

Figure S7. Net impacts (production minus recycling benefits) with varying recycling quota (share of cells for which recycling benefit is accounted for). The underlying values are provided in a separate ESI document in Excel format.

The importance of a high recycling quota becomes evident especially under ADP (resource depletion) and HTP (human toxicity) aspects. Here, only for recycling quota close to 100% can the LIB (but also the NaNMC) achieve results that are competitive to ore even better that those of the remaining SIB. For lower recycling quota, the benefit of recycling (which is especially high for the LIB and NaNMC cells) decreases much stronger for these battery cells, giving advantages to the SIB based on abundant materials like the NaMMO, NaPBA, abut also NaNMMT cells.

6.5. Impact assessment, all impact categories

The results of the impact assessment for the manufacturing and the recycling stage are provided in Figure S8

per kWh	Abbr	NaNMC Prod	NaNMC Rec	NaNMC Net	NaMVP Prod	NaMVP Rec	NaMVP Net
Acidification	**AP**	0.99028828	-0.61787217	0.372416105	0.85528021	-0.21498743	0.64029278
Climate change	**GWP**	86.6528142	-31.8993722	54.753442	89.6514007	-8.32172376	81.3296769
Freshwater ecotoxicity	**ETP_f**	3473.24975	-2279.06497	1194.184771	2377.38481	-283.08696	2094.29785
Freshwater eutrophication	**EP_f**	0.03113995	-0.00953779	0.021602155	0.03666208	-0.00031188	0.0363502
Human toxicity, cancer effects	**HTP_c**	3.8929E-05	-2.7655E-05	1.12744E-05	9.5141E-05	-2.5604E-06	9.2581E-05
Human toxicity, non-cancer ef	**HTP_{nc}**	7.6974E-05	-5.1756E-05	2.52179E-05	7.915E-05	-1.6912E-06	7.7459E-05
Ionizing radiation E (interim)	**IRPe**	0.00015876	-0.00010595	5.28128E-05	2.9823E-05	1.815E-06	3.1638E-05
Ionizing radiation HH	**IRP_{hh}**	25.9884667	-13.273577	12.71488969	9.02783159	1.27200373	10.2998353
Land use	**LU**	94.8495689	-35.1835947	59.66597425	116.679808	-10.4632687	106.216539
Marine eutrophication	**EP_m**	0.15614189	-0.11053734	0.04560455	0.12803331	-0.05275301	0.07528031
Mineral, fossil & ren resource	**ADP**	0.03619308	-0.0282344	0.007958689	0.00782461	-0.0039123	0.0039123
Ozone depletion	**ODP**	1.1543E-05	-4.017E-06	7.52562E-06	7.7831E-06	-6.5082E-07	7.1323E-06
Particulate matter	**PMP**	0.07314414	-0.04352013	0.029624008	0.06688778	-0.0150182	0.05186958
Photochemical ozone formatic	**POF**	0.36527855	-0.2224643	0.142814249	0.36611597	-0.10216162	0.26395434
Terrestrial eutrophication	**EP_t**	1.4475339	-0.96098009	0.486553809	1.30330216	-0.52456429	0.77873787
Water resource depletion	**WDP**	99.0620524	-51.6215716	47.44048076	43.9984057	-2.87541749	41.1229882

per kWh	Abbr	NaMMO Prod	NaMMO Rec	NaMMO Net	NaNMMT Prod	NaNMMT Rec	NaNMMT Net	NaPBA Prod	NaPBA Rec	NaPBA [illegible]
Acidification	**AP**	0.49857514	-0.29174101	0.20683414	0.52978018	-0.33576728	0.1940129	0.57322963	-0.2816283	0.29
Climate change	**GWP**	52.3353545	-6.33946002	45.9958945	50.5991821	-13.3393018	37.2598803	87.0472935	-13.1097033	73.9
Freshwater ecotoxicity	**ETP_f**	777.686189	-211.774214	565.911975	1282.92082	-584.353151	698.567672	1310.47112	-459.927868	850
Freshwater eutrophication	**EP_f**	0.01756258	0.00026079	0.01782337	0.01640968	-0.00258768	0.013822	0.02496393	-0.00163081	0.02
Human toxicity, cancer effects	**HTP_c**	6.0965E-06	-1.9498E-06	4.1468E-06	1.0232E-05	-5.9023E-06	4.3294E-06	1.0225E-05	-4.1152E-06	6
Human toxicity, non-cancer ef	**HTP_{nc}**	1.1274E-05	-1.0297E-06	1.0244E-05	1.9225E-05	-9.3046E-06	9.9202E-06	1.6905E-05	-3.6474E-06	1.3
Ionizing radiation E (interim)	**IRPe**	2.2441E-05	9.29E-07	2.337E-05	3.6197E-05	-1.6287E-05	1.991E-05	2.7914E-05	1.3785E-06	2.9
Ionizing radiation HH	**IRP_{hh}**	7.43933246	1.07662413	8.51595658	8.35732329	-1.55803591	6.79928738	9.27115348	1.2369692	10.5
Land use	**LU**	58.556425	-11.5655914	46.9908336	71.7097923	-28.196499	43.5132934	77.0587719	-14.796776	62.2
Marine eutrophication	**EP_m**	0.09760499	-0.06026871	0.03733628	0.0994679	-0.06614363	0.03332427	0.11967635	-0.06134354	0.05
Mineral, fossil & ren resource	**ADP**	0.00530668	-0.00385366	0.00145302	0.00908844	-0.00612207	0.00296637	0.0080286	-0.005896	0.0
Ozone depletion	**ODP**	4.6715E-06	-9.5028E-07	3.7212E-06	4.6526E-06	-1.3223E-06	3.3303E-06	8.8869E-06	-7.3743E-07	8.1
Particulate matter	**PMP**	0.04156899	-0.01610956	0.02545943	0.03547015	-0.02076456	0.0147056	0.04754438	-0.02120053	0.02
Photochemical ozone formatic	**POF**	0.2294507	-0.12565458	0.10379612	0.22102575	-0.13285529	0.08817047	0.28438813	-0.13197014	0.15
Terrestrial eutrophication	**EP_t**	1.05463931	-0.65461678	0.40002253	0.97195791	-0.6494446	0.32251331	1.20341216	-0.65370382	0.54
Water resource depletion	**WDP**	31.5883237	-1.78260198	29.8057217	35.2248276	-10.9380609	24.2867667	47.8567396	-6.7314809	41.1

per cell	Abbr	NaNMC Prod	NaNMC Rec	NaNMC Net	NaMVP Prod	NaMVP Rec	NaMVP Net
Acidification	AP	0.15678	-0.09782	0.05896	0.13554	-0.03407	0.10147
Climate change	GWP	13.71866	-5.05023	8.66843	14.20745	-1.31878	12.88867
Freshwater ecotoxicity	ETP_f	549.87634	-360.81595	189.06039	376.75458	-44.86203	331.89255
Freshwater eutrophication	EP_f	0.00493	-0.00151	0.00342	0.00581	-4.9425E-05	0.00576058
Human toxicity, cancer effects	HTP_c	6.1632E-06	-4.3782E-06	1.78494E-06	1.5077E-05	-4.0576E-07	1.4672E-05
Human toxicity, non-cancer ef	HTP_{nc}	1.2186E-05	-8.194E-06	3.99244E-06	1.2543E-05	-2.68E-07	1.2275E-05
Ionizing radiation E (interim)	IRPe	2.5135E-05	-1.6774E-05	8.3612E-06	4.7261E-06	2.8764E-07	5.0138E-06
Ionizing radiation HH	IRP_{hh}	4.11443	-2.10144	2.01299	1.43068	0.20158	1.63226
Land use	LU	15.01635	-5.57018	9.44617	18.49076	-1.65816	16.8326
Marine eutrophication	EP_m	0.02472	-0.0175	0.00722	0.02029	-0.00836	0.01193
Mineral, fossil & ren resource	ADP	0.00573	-0.00447	0.00126	0.00124	-0.00062	0.00062
Ozone depletion	ODP	1.8274E-06	-6.3596E-07	1.19144E-06	1.2334E-06	-1.0314E-07	1.1303E-06
Particulate matter	PMP	0.01158	-0.00689	0.00469	0.0106	-0.00238	0.00822
Photochemical ozone formatic	POF	0.05783	-0.03522	0.02261	0.05802	-0.01619	0.04183
Terrestrial eutrophication	EP_t	0.22917	-0.15214	0.07703	0.20654	-0.08313	0.12341
Water resource depletion	WDP	15.68326	-8.1726	7.51066	6.97262	-0.45568	6.51694

per cell	Abbr	NaMMO Prod	NaMMO Rec	NaMMO Net	NaNMMT Prod	NaNMMT Rec	NaNMMT Net	NaPBA Prod	NaPBA Rec	
Acidification	AP	0.07892	-0.04618	0.03274	0.08394	-0.0532	0.03074	0.09139	-0.0449	
Climate change	GWP	8.28422	-1.00348	7.28074	8.01709	-2.11352	5.90357	13.87795	-2.09008	1
Freshwater ecotoxicity	ETP_f	123.10079	-33.52197	89.57882	203.26992	-92.58671	110.68321	208.92841	-73.3263	13
Freshwater eutrophication	EP_f	0.00278	0.00004128	0.00282128	0.0026	-0.00041	0.00219	0.00398	-0.00026	
Human toxicity, cancer effects	HTP_c	9.6503E-07	-3.0863E-07	6.564E-07	1.6211E-06	-9.3517E-07	6.8596E-07	1.6302E-06	-6.5608E-07	9.7
Human toxicity, non-cancer ef	HTP_{nc}	1.7846E-06	-1.6299E-07	1.6216E-06	3.046E-06	-1.4743E-06	1.5718E-06	2.6951E-06	-5.8151E-07	2.1
Ionizing radiation E (interim)	IRPe	3.5523E-06	1.4705E-07	3.6993E-06	5.7351E-06	-2.5805E-06	3.1546E-06	4.4503E-06	2.1977E-07	4.6
Ionizing radiation HH	IRP_{hh}	1.17758	0.17042	1.348	1.32416	-0.24686	1.0773	1.4781	0.19721	
Land use	LU	9.26896	-1.83073	7.43823	11.36192	-4.46754	6.89438	12.28548	-2.35905	
Marine eutrophication	EP_m	0.01545	-0.00954	0.00591	0.01576	-0.01048	0.00528	0.01908	-0.00978	
Mineral, fossil & ren resource	ADP	0.00084	-0.00061	0.00023	0.00144	-0.00097	0.00047	0.00128	-0.00094	
Ozone depletion	ODP	7.3946E-07	-1.5042E-07	5.8904E-07	7.3717E-07	-2.095E-07	5.2767E-07	1.4168E-06	-1.1757E-07	1.2
Particulate matter	PMP	0.00658	-0.00255	0.00403	0.00562	-0.00329	0.00233	0.00758	-0.00338	
Photochemical ozone formatic	POF	0.03632	-0.01989	0.01643	0.03502	-0.02105	0.01397	0.04534	-0.02104	
Terrestrial eutrophication	EP_t	0.16694	-0.10362	0.06332	0.154	-0.1029	0.0511	0.19186	-0.10422	
Water resource depletion	WDP	5.00015	-0.28217	4.71798	5.58113	-1.73306	3.84807	7.6298	-1.0732	

Figure S8. Characterization results for all impact categories. Numerical values are provided in a separate ESI document in Excel format.

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