# Exploring the Economic Potential of Sodium-Ion Batteries

**Jens F. Peters[1,2], Alexandra Peña Cruz[1,2] and Marcel Weil[1,2,3]**

[1]Helmholtz Institute Ulm (HIU), Helmholtzstr. 11, 89081 Ulm (Germany)

[2] Karlsruhe Institute of Technology (KIT), P.O.Box 3640, 76021 Karlsruhe, Germany

[3] ITAS, Institute for Technology Assessment and Systems Analysis, 76021 Karlsruhe, Germany

** SUPPLEMENTARY INFORMATION **

This Supplementary Information contains detailed information about the underlying calculation methods, price assumptions, and data sources, and the cell dimensioning realized for determining the battery cell mass balances.

**Price adjustment**

Prices in this work are (unless stated otherwise) provided in € (2017). Values for other years are adapted to 2017 according to the currency exchange rates and the Industrial Producer Price Index (IPP) for Germany [1–3], as provided in Table S1.

**Table S1.** IPP and exchange rate for 2010–2017.

| Type | Unit | 2008 | 2009 | 2010 | 2011 | 2012 | 2013 | 2014 | 2015 | 2016 | 2017 |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **Exchange rate** | €/$ | 0.683 | 0.719 | 0.755 | 0.719 | 0.778 | 0.753 | 0.754 | 0.902 | 0.904 | 0.887 |
| **IPP (2010)** | % | 99.0 | 97.0 | 100.0 | 103.0 | 104.7 | 104.2 | 104.1 | 105.0 | 104.0 | 105.3 |

**Cathode Active Material**

The prices for the cathode active materials were estimated via the average market prices of the contained metals according to Equation (S1) [4]. Although some price estimations for NMC and LFP materials were found in the literature, an explicit calculation was needed for the NMMT SIB cathode material. Thus, the NMC material was also calculated in the same way in order to have a common basis for comparison. Additionally, comparing the obtained NMC price with the prices that were found in the literature allowed for a certain validation of the cost model for the layered oxide active materials.

$$C = C_0 + \frac{1}{MW} * \sum_i x_i * C_i * MW_i \qquad \text{Equation (S1)}$$

*Where:*

*$C$ = Active material cost (€/kg)*
*$C_0$ = Baseline cost (€)*
*$C_i$ = Price of raw materials i (€/kg)*
*$x_i$ = Molar stoichiometry (-)*
*$MW_i$ = Molecular weight of the raw material (g/mol)*
*$MW$ = Molecular weight of the product / active material (g/mol)*

The baseline cost (C0) is the part of the active material cost not associated with the required raw materials, that is, the cost of processing, depreciation, and overheads of the manufacturing process. For co-precipitated metal oxides such as NMC333, the baseline cost is 9.04 €/kg [4]. Because NMMT is similar in nature to NMC333, the cathode processing of the lithium-ion and the sodium-ion active materials was assumed to be the same, and so was their baseline cost. Since no information about the baseline cost of phosphate compounds (such as LFP) was found in the literature, Equation (S1) could not be applied readily to this material. For this reason, for the cost of the LFP, an average value from different literature sources was taken instead [4–7]. For the sensitivity analysis and discussion, an alternative LFP price was calculated using the same baseline costs as for the layered oxide materials.

The prices for the raw materials (Ci) were partially obtained from the literature and geological surveys [7]. However, for some precursor materials, only prices obtained from a laboratory were available, which were excessively high for this work. For these materials, the prices were estimated based on the average market prices of the contained metals and the stoichiometric amount of metal required for their (hypothetical) synthesis according to Equation (S2).

$$C_i = \frac{C_M * MW_M * n}{MW_i} \quad \text{Equation (S2)}$$

*Where:*

*$C_i$ = Price of the precursor material (€/kg)*
*$C_M$ = Price of the metal (€/kg)*
*$MW_M$ = Molar weight of the metals (g/mol)*
*$MW_i$ = Molar weight of the precursor material (g/mol)*
*n = Moles of the raw materials (mol)*

The final prices of the precursor material calculated via Equation (S2) are displayed in Table S2.

**Table S2.** Prices of metals and other components according to USGS [7]. 10-year average refers to the average metal price 2007–2017. Source S2 = calculated via Equation (S2). Min and max prices are given only for the metals considered in the sensitivity analysis.

| **Metals** | **Price $C_i$ (€/kg) 2007–2017 average** | **Price (€/kg) 2007–2017 min** | **Price (€/kg) 2007–2017 max** | **Source** |
|---|---|---|---|---|
| Nickel (Ni) | 16.31 | 10.48 | 33.61 | [8] |
| Magnesium (Mg) | 2.53 | | | [8] |
| Manganese (Mn) | 0.55 | | | [8] |
| Cobalt (Co) | 38.25 | 23.11 | 77.71 | [8] |
| Iron/Steel (Fe) | 0.17 | | | [8] |
| Copper (Cu) | 6.05 | 4.43 | 7.95 | |
| $Li_2CO_3$ | 6.93 | 4.68 | 12.56 | [8] |
| $MnSO_4$ | 0.47 | | | S2 |
| $NiSO_4$ | 6.19 | 3.98 | 12.75 | S2 |
| $CoSO_4$ | 14.54 | 8.79 | 29.55 | S2 |
| $Na_2CO_3$ | 0.11 | | | [8] |
| $MnO_2$ | 0.35 | | | S2 |
| $NiCO_3$ | 8.06 | 5.18 | 16.62 | S2 |
| $Mg(OH)_2$ | 1.05 | | | S2 |
| $TiO_2$ | 3.34 | | | [8] |

The stoichiometry ($x_i$) required by Equation (S1) is provided, together with the precursor materials required for the cathode materials synthesis in Table S3, obtained from the chemical formula of every positive active material (see Table S3). After collecting the information, the price of the lithium-ion and sodium-ion cell cathode active materials was calculated.

**Table S3.** Precursor materials for the cathode active material synthesis.

| Cathode Active Materials | MW (g/mol) | Precursor Materials [1,18] |
|---|---|---|
| **$NMC_{333}$** ($Li_{1.05}Ni_{0.33}Mn_{0.33}Co_{0.33}O_2$) [4,8,9] | 95.88 | Lithium carbonate ($Li_2CO_3$)<br>Manganese (II) sulfate ($MnSO_4$)<br>Nickel(II) sulfate ($NiSO_4$)<br>Cobalt(II) sulfate ($CoSO_4$) |
| **NMMT** ($Na_{1.1}Ni_{0.3}Mn_{0.5}Mg_{0.05}Ti_{0.05}O_2$) [10,11] | 105.97 | Sodium Carbonate ($Na_2CO_3$)<br>Manganese dioxide ($MnO_2$)<br>Nickel (II) carbonate ($NiCO_3$)<br>Magnesium hydroxide ($Mg(OH)_2$ )<br>Titanium dioxide ($TiO_2$) |

**Electrolyte**

The composition of the electrolytes was calculated for a 1 M solution of $LiPF_6$ / $NaPF_6$ salt in an 80/20% mixture of ethylene carbonate (EC) and dimethyl carbonate (DMC) as provided in Table S4.

**Table S4.** Composition of the electrolytes used for the SIB and LIB.

| LIB | Per liter | Per kg | | SIB | Per liter | Per kg | |
|---|---|---|---|---|---|---|---|
| **EC** | 1.040 | 0.74 | kg | **EC** | 1.040 | 0.73 | kg |
| **DMC** | 0.214 | 0.15 | kg | **DMC** | 0.214 | 0.15 | kg |
| **$LiPF_6$** | 0.152 | 0.11 | kg | **$NaPF_6$** | 0.168 | 0.12 | kg |
| **Total** | 1.406 | 1.00 | kg | **Total** | 1.422 | 1.00 | kg |

The amount of $Li_2CO_3$ / $Na_2CO_3$ required per kg of electrolyte was then calculated based on stoichiometry (52.5g $Li_2CO_3$/74.5g $Na_2CO_3$). With the known average price of $Li_2CO_3$ (Table S3) and an average market price of 16.06 €/l [4], the contribution of the $Li_2CO_3$ to the total electrolyte cost was then estimated and thus, by substituting the $Li_2CO_3$ with $Na_2CO_3$, the price for the SIB electrolyte (15.84€/l).

**Battery Composition**

The dimensioning of the battery cells was done based on technical datasheets for LIB and SIB [12]. These allowed for a detailed estimation of the active material surfaces and thus also the volume of required electrolyte. From the data provided in the datasheets, an active material void fraction was calculated based on the ratio between the density of the coating and the density of the bulk active materials. The total electrolyte volume required was then calculated based on the inner volume of the 18650 cell can, the volumes of electrodes and separator, and the electrode active material void (pore volume). The principal parameters used for calculating the mass balances are provided in Table S5. Table S6 contains the obtained mass balances per single 18650 cells, both for the "own" dimensioning based on Table S7 and with alternative mass balances taken directly from published literature (the corresponding references are given directly within the table).

**Table S5.** Cell dimensioning parameters used for the base case assessment, based on technical datasheets from Faradion [12].

| Parameter | NMMT | NMC | LFP | Unit |
|---|---|---|---|---|
| ElectrodeWidthAnode | 60 | 60 | 60 | mm |
| ElectrodeWidthCathode | 60 | 60 | 60 | mm |
| CoatThickness Anode (single side) | 0.125 | 0.08 | 0.06 | mm |
| CoatThickness Cathode (single side) | 0.082 | 0.082 | 0.082 | mm |
| ActMatLengthAnode1stcoat | 460 | 606 | 650 | mm |
| ActMatLengthAnode2ndcoat | 420 | 566 | 610 | mm |
| ActMatLengthCathode1stcoat | 430 | 545 | 624 | mm |

| | | | | |
|---|---|---|---|---|
| ActMatLengthCathode2ndcoat | 410 | 525 | 604 | mm |
| Anode collector foil thickness | 0.02 | 0.015 | 0.015 | mm |
| Cathode collector foil thickness | 0.02 | 0.02 | 0.02 | mm |
| CoatingAnode | 0.177 | 0.104 | 0.078 | $mg/mm^2$ |
| CoatingCathode (incl. binder / additives) | 0.265 | 0.260 | 0.176 | $mg/mm^2$ |
| Collector foil overlap | 1 | 1 | 1 | mm |
| Collector foil width anode | 480 | 625 | 670 | mm |
| Collector foil width cathode | 470 | 585 | 664 | mm |
| Separator overlap height | 1 | 1 | 1 | mm |
| Separator overlap length | 7 | 7 | 7 | mm |
| Separator thickness | 0.023 | 0.023 | 0.023 | mm |
| Collector foil density anode | 2.7 | 8.96 | 8.96 | $g/cm^3$ |
| Collector foil density cathode | 2.7 | 2.7 | 2.7 | $g/cm^3$ |
| Cathode density (calculated) | 2.94 | 2.60 | 2.15 | $g/cm^3$ |
| Cathode material void (calculated) | 0.32 | 0.32 | 0.33 | |
| Anode density (calculated ) | 1.48 | 1.53 | 1.56 | $g/cm^3$ |
| Anode material void (calculated) | 0.38 | 0.40 | 0.43 | |
| Mass fraction of active material in cathode | 0.95 | 0.95 | 0.95 | |
| Mass fraction of active material in anode | 0.95 | 0.95 | 0.95 | |
| Electrolyte volume | 5.31 | 5.19 | 5.09 | $cm^3$ |

**Table S6.** Mass balance by cell components for the battery cells based on different literature sources. "Own" indicates the base case model with cell dimensioning according to Table S5.

| **Component** | **Sub-component** | **Unit** | **NMMT** | | | **NMC** | | | | **LFP** | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | **own** | [12] | [13] | **own** | [8] | [9] | [14] | **own** | [8] | [15] | [14] |
| Anode | Active material | g | 8.88 | 8.88 | 8.34 | 6.94 | 5.32 | 5.97 | 6.20 | 5.60 | 4.53 | 6.45 | 5.20 |
| | Conductive carbon | g | 0.19 | 0.19 | 0.28 | 0.15 | | | | 0.12 | | | |
| | Binder | g | 0.25 | 0.25 | 0.36 | 0.20 | 0.28 | | | 0.16 | 0.24 | 0.77 | |
| | Collector foil | g | 1.56 | 1.56 | 1.46 | 5.04 | 4.95 | 7.92 | 7.50 | 5.40 | 4.95 | 1.76 | 3.90 |
| Cathode | Active material | g | 12.69 | 12.69 | 12.03 | 15.86 | 12.03 | 13.63 | 11.30 | 12.32 | 12.86 | 16.11 | 9.70 |
| | Conductive carbon | g | 0.21 | 0.21 | 0.24 | 0.26 | 0.69 | | | 0.20 | 0.74 | | |
| | Binder | g | 0.43 | 0.43 | 0.53 | 0.53 | 1.11 | | | 0.41 | 1.18 | 0.99 | |
| | Collector foil | g | 1.52 | 1.52 | 1.30 | 1.90 | 2.15 | 1.69 | 3.10 | 2.15 | 2.15 | 0.73 | 2.10 |
| Separator | Separator | g | 0.78 | 1.13 | 0.81 | 0.97 | 1.97 | 0.78 | 1.40 | 1.15 | 1.97 | 0.69 | 1.20 |
| Electrolyte | Electrolyte | g | 7.56 | 7.51 | 5.67 | 6.62 | 7.15 | 5.70 | 4.40 | 7.13 | 7.15 | 7.06 | 6.40 |
| Housing | 18650 Cell container | g | 9.30 | 9.30 | 9.32 | 9.30 | 9.30 | 9.30 | 9.20 | 9.30 | 9.30 | 9.30 | 10.50 |
| | Sealing | g | 0.20 | 0.20 | 0.20 | 0.20 | | | | 0.20 | | | |
| **Parameter** | | **Unit** | | | | | | | | | | | |
| Cell mass | | g | 43.56 | 43.87 | 40.54 | 47.96 | 44.94 | 45.00 | 43.10 | 44.08 | 45.06 | 43.85 | **39.00** |
| Energy density | | Wh | 6.09 | | | 9.97 | | | | 6.31 | | | |

**Cell Energy Density**

For the calculation of the energy density of the battery cells, the average gravimetric energy densities of commercial active materials was used as given in Table S7 [12,16].

**Table S7.** Parameters used for the calculation of the battery cell energy density.

| **Active material** | **Energy density (mAh/g)** | **Voltage (V)** |
|---|---|---|
| $NMC_{333}$ | 170 | 3.7 |
| LFP | 125 | 3.2 |
| NMMT | 150 | 3.2 |
| Graphite | 300 | -- |
| Hard carbon | 240 | -- |

**Battery Cell Manufacturing**

The final battery cell price depends on the costs for the battery materials, running costs for the manufacturing plant, investment costs, and overhead costs such as insurance, in addition to profit margins. For determining the price of the final battery cell, the BatPaC V3.0 calculation tool provided by ANL was modified and adjusted to the manufacturing of 18,650 round cells (the original BatPaC is oriented towards the dimensioning of automotive battery packs according to requirements regarding mileage and power and assumes prismatic battery cells). For this purpose, the parameters that were specific for prismatic cells were modified and adjusted to round cells according to the data provided by Ciez and Whitacre [17]. The parameters included specifically receiving, inter-process materials handling, electrode processing, slitting and vacuum drying, control laboratory, cell assembly and cell formation, sealing, and testing, rejected cell and scrap recycle, and shipping. The annual throughput of the plant in terms of kWh/y, an important cost factor (economy of scale), was maintained similar to the one used by BatPaC for the baseline plant. However, due to the different capacities of 18650 round cells and prismatic cells, the throughput in terms of cells per year increased significantly, which also explains why the costs that account on a per cell basis (e.g., cell filling, cycling, and formation) changed correspondingly. Therefore, 85 Mio round cells are produced per year, equivalent to 518,000 kWh/y for the SIB and 666,000 kWh/y for the NMC battery.

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