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Life cycle assessment of lithium nickel cobalt manganese oxide (NCM) batteries for electric passenger vehicles

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13 Abstract

14 This study evaluated and quantified the life cycle environmental impacts of lithium-ion power batteries (LIBs) 15 for passenger electric vehicles to identify key stages that contribute to the overall environmental burden and to find 16 ways to reduce this burden effectively. Primary data for the assessment were collected onsite from the one Chinese 17 leading LIB supplier, two leading cathode material producers and two battery recycling corporations from 2017 to 18 2019. Six environmental impact categories, including primary energy demand (PED), global warming potential 19 (GWP), acidification potential (AP), photochemical oxidant creation potential (POCP), eutrophication potential (EP) 20 and human toxicity potential (HTP), were considered in accordance with the ISO 14040/14044 standards. 21 The results indicate that material preparation stage is the largest contributor to the LIB's life cycle PED, GWP, 22 AP, POCP, EP and HTP, with the cathode active material, wrought aluminum and electrolytes as the predominant 23 contributors. In the production stage, vacuum drying and coating and drying are the two main processes for all the 24 six impact categories. In the end-of-life stage, waste LIBs recycling could largely reduce the life cycle POCP and 25 HTP. 26 Sensitivity analysis results depict that optimizing the mass of cathode active material and wrought aluminum

27 could effectively reduce the environmental impacts of the LIB, but the recycling benefits could vary with impact 28 categories and with life cycle stages. We hope this study is helpful to reduce the uncertainties associated with the 29 life cycle assessment of LIBs in existing literatures and to identify opportunities to improve the environmental 30 performance of LIBs within the whole life cycle.

31 Keywords Lithium-ion power battery; Battery electric vehicle; Life cycle assessment; Battery recycling

33 1 Introduction

34 To save energy and reduce environmental emissions from the automotive industry, the Chinese government has 35 launched numerous policies and programs to promote new energy vehicles (NEVs), which include battery electric 36 vehicles (BEVs), plug-in hybrid electric vehicles (PHEVs), and fuel cell electric vehicles (FCVs). In 2009, China 37 launched the "Ten Cities and Thousand Vehicles" project to promote NEVs. From 2009 to 2012, a total of 17,000 38 NEVs were promoted (MOST et al., 2009). Since 2014, China has been in the stage of large-scale promotion and 39 application of NEVs. In 2018, the cumulative sales of NEVs reached 3.0 million, accounting for more than 53% of 40 global cumulative sales (Wan, 2019). China has become the world's largest market for NEVs. By the end of 2019, 41 the stock of NEVs reached 3.8 million, accounting for 1.5% of the total vehicles in China (Jiang, 2020). 42 As the core component of NEVs, the capacity of power batteries has also increased by a significant amount 43 each year. China has been the world's largest power battery producer (MIIT, 2017). The cumulative installed 44 capacity of power batteries in China reached 144 GWh by the end of 2018, which represents the largest power 45 battery market worldwide (MIIT, 2019). 46 Currently, lithium-ion power batteries (LIBs), such as lithium manganese oxide (LiMn₂O₄, LMO) battery, 47 lithium iron phosphate (LiFePO₄, LFP) battery and lithium nickel cobalt manganese oxide (LiNi_xCo_yMn_zO₂, NCM) 48 battery, are widely used in BEVs in China. According to the data from China Automotive Technology and Research 49 Center Co., Ltd, NCM batteries accounted for 42% of the cumulative installed capacity of power batteries and 77% 50 of the cumulative installed capacity of passenger BEVs until 2018 in China. Current types of NCM batteries in 51 Chinese market include old-fashioned NCM 111 (LiNi_{1/3}Mn_{1/3}Co_{1/3}O₂), state-of-art NCM 622 (LiNi_{0.6}Mn_{0.2}Co_{0.2}O₂) 52 and upcoming technology NCM 811 (LiNi_{0.8}Mn_{0.1}Co_{0.1}O₂) while NCM 622 batteries have been the most commonly 53 used in electric passenger vehicles in China (CATARC and BIT, 2019). 54 NEV sales will maintain long-term growth in China benefiting from various policy supports. The "Technology 55 Roadmap For Energy Saving And New Energy Vehicles" (TRESNEV Steering Committee China-SAE, 2016) shows 56 that the total sales of NEVs is forecasted to exceed 5 million in 2025 and 15 million in 2030. This projection will

57 lead to a huge number of demand and disposal of power batteries in China in the near future.

With the fast expansion of NEVs, China will be facing with challenges of waste power battery recycling and
disposal. The capacity of decommissioned power batteries was 1.2 GWh in 2018 in China, and it is expected to be

more than 200,000 tons by 2020, which indicates that about 25 GWh of power batteries need to be recycled and
reused by 2020 (MIIT, 2019).

The environmental impacts associated with LIBs within the life cycle are key challenges that restrict the sustainable development of NEVs. First, LIBs contain various types of valuable metal materials, which can produce large amount of pollutants in the exploitation and extraction stages. In addition, the assembly process of LIBs can be energy intensive (Dai et al., 2019; Ellingsen et al., 2017). Finally, the improper recycling and waste disposal processes may incur negative environmental pollutions and human toxicity. Therefore, an environmental assessment is required to quantify the overall environmental impacts of LIBs in BEVs application from a full life cycle perspective.

To address the gaps in environmental aspects of LIBs production and promote NEVs development in China. In this study, we aim to quantify the life cycle environmental impacts of NCM 622 batteries for electric passenger vehicles using the primary data collected from the latest and representative onsite investigations in China covering material production, LIB production and battery recycling plants. Inventory data is also supplemented by Ecoinvent 3.0, GREET 2018 database (ANL GREET, 2018) where available. The results can help identify the key contributors to the LIB life cycle environmental impacts and propose strategies to reduce these impacts effectively.

75 2 Literature review

76 Life cycle assessment (LCA) is a tool to assess the potential environmental impacts and resources used 77 throughout a product's life cycle, i.e., from material preparation, via production and use phases, to waste 78 management (ISO, 2006). Until now, there have been several LCA studies of LIBs. Notter et al. (2010) conducted 79 an early LCA study of LMO batteries and the contributions to the environmental burden caused by different battery 80 materials were analyzed. USEPA (2013) conducted a LCA study to bring together and use life cycle inventory data 81 directly provided by LIB suppliers, manufacturers, and recyclers. (Ellingsen et al., 2014) studied the cradle-to-gate 82 environmental impacts of NCM batteries by using midpoint indicators, which include 13 impact categories. Kim et 83 al. (2016) chose a commercial BEV and assessed the life cycle greenhouse gas (GHG) emissions and other air 84 emissions of traction batteries.

85 In addition, other scientists have provided richer perspectives and deeper discussions. MajeauBettez et al.
86 (2011) compared the environmental impacts of three different LIBs, NCM, NiMH, and LFP batteries, during

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87 production and operation phases. They concluded that NiMH batteries have the highest environmental burden, 88 followed by NCM and then LFP. Li et al. (2014) and Deng et al. (2017) reported the environmental impacts of next-89 generation LIBs compared with conventional LIBs to support the selection and development of future LIBs. 90 Ellingsen et al. (2017) pointed out that both Notter et al. (2010) and Dunn et al. (2012) neglected processes in cell 91 manufacturing and therefore underestimated the energy demand. Ellingsen et al. (2017) indicated that USEPA 92 (2013) reported very different energy use associated with cell manufacturing and pack assembly for NCM, LFP, and 93 LMO batteries without clear explanations. Peters et al. (2017) provided a review of LCA studies on LIB and found 94 that only a few publications contributed original life cycle inventory (LCI) data. Peters et al. (2017) pointed that the 95 majority of existing studies focus on GHG emissions or energy demand only, while the impacts in other categories 96 such as toxicity might be even more important. Dai et al. (2019) analyzed the cradle-to-gate energy use, GHG 97 emissions, SO_x, NO_x, PM₁₀ emissions, and water consumption associated with current industrial production of NCM 98 batteries. Dai et al. (2019) pointed out that the existing LCA studies of LIB, including the studies conducted by 99 Notter et al. (2010), MajeauBettez et al. (2011), Dunn et al. (2012) and (Ellingsen et al., 2014) were carried out 100 when automotive LIBs were at their early commercialization stage which might be different from current practices. 101 Besides, Dai et al. (2019) also identified knowledge gaps, such as the LCI data for graphite, $LiPF_{6}$, and the 102 separator, which should be improved in future studies. 103 Moreover, some studies have deeply discussed the environmental impacts during the recycling process of LIBs. 104 (Dunn et al., 2012) calculated the energy consumed and the air emissions generated when recycling LMO batteries 105 in the U.S. and estimated that direct recycling could avoid 48% energy consumption associated with primary 106 material production. (Hendrickson et al., 2015) distinguished hydrometallurgical and pyrometallurgical recycling 107 methods of LMO, LFP, and NCM batteries, and the results showed that hydrometallurgy achieves greater energy 108 savings. 109 Although several LCA studies assessed LIBs, they presented significantly different results with large 110 uncertainties associated with data and results (Dai et al., 2019; Ellingsen et al., 2017; Peters et al., 2017). First, for 111 the background data, most of these studies used secondary LCI databases, disunified LCI databases, or literature 112 publications as data sources. In addition, for the foreground data, most studies were conducted based on previous 113 literature publications, engineering calculations and secondary data, and therefore did not reflect the current

114 commercial-scale automotive LIB production. Furthermore, for the life cycle stages, most studies only focused on

115 production (cradle-to-gate), while only a few have clearly assessed the end-of-life stage. Therefore, it is essential to

assess the life cycle environmental impacts of LIBs with primary life cycle data in the context of China and identify

117 the potential for reducing the environmental impacts of LIBs.

118 3 Methods

119 **3.1** Goal and scope

The goal of this study is to assess the environmental impacts of NCM batteries within the battery life cycle and to identify the key contributory processes exploring improvement opportunities. In this study, the functional unit is defined as 1 kWh of the NCM 622 pack for a passenger BEV. As shown in Figure 1, the system boundaries cover the life cycle stages of the LIB, including material preparation, production and end-of-life stages. The use stage is excluded in the LIB's system boundaries due to the large uncertainty of some key parameters, such as the real world driving cycles, different charging behaviors, battery replacement times, and the lack of unified allocation method of the electricity consumption of the battery pack.

This study was conducted in accordance with the principles of the ISO 14040 series standards for LCA.(ISO,
2006) SimaPro 8 software (PRé Sustainability, Netherlands) was used as a support tool to establish the LCA model
and perform the impact assessment.

130 **3.2 Methods and databases**

To collect the cradle to grave primary LCI data, this study conducted onsite investigations in six leading LIB factories (with a total China market share of over 75% in 2018), five leading LIB material producer and two battery recycling corporations from 2017 to 2019 in China. Considering the representative and completeness of the onsite data, this study chose the primary data from two Chinese leading LIB suppliers (world's top three), two leading cathode material producer (world's top five), and two battery recycling corporation (one owned by the world's top three LIB supplier, and the other one is the world's leading waste battery and cobalt nickel tungsten rare metal recycling corporation). A sensitivity analysis has been conducted to evaluate the data uncertainties.

138 The upstream materials and energy flows for NCM 622 precursor and NCM 622 production were obtained 139 from onsite investigations of two leading cathode material producer in 2018 in China, which are of the world's top 140 five NCM suppliers (Tables S 2 and S 3). For the LCI data of dimethyl carbonate (DMC), polyvinylidene fluoride

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- 141 (PVDF) and electronic parts, the foreground data were acquired from the GREET 2018 (Greenhouse Gases,
- 142 Regulated Emissions, and Energy Use in Transportation) model,(ANL GREET, 2018). The background data were
- primarily based on the China Automotive Life Cycle Database (CALCD) (Sun et al., 2015; Sun et al., 2017) with
- 144 Ecoinvent 3.0 database as supplements. The CALCD, a local Chinese LCI database developed by the China
- 145 Automotive Technology and Research Center, is a process-based life cycle database. Detailed data source
- 146 information is listed in Table S 1, Table S 2 and Table S 3 in the Supporting Information.
- 147 The CML-IA baseline V3.02 method developed by the Institute of Environmental Sciences of Leiden
- 148 University is selected as the base method. Six impact categories, including primary energy demand (PED), global
- 149 warming potential (GWP), acidification potential (AP), photochemical oxidant creation potential (POCP),
- 150 eutrophication potential (EP) and human toxicity potential (HTP) are chosen from this approach to assess the impact
- 151 characterization results, and these categories are easily communicated, of general interest, and important with
- 152 respect to LIBs. As a comparison, ReCiPe Midpoint (H) V1.11 / World Recipe H method is applied to present ten
- 153 impact categories. The normalization and weighting phases are not included in this study.
- 154 **3.3 Life cycle inventory analysis**

155 3.3.1 Material preparation

156 For the investigated NCM 622 pack in this study, which is used by one passenger car, the pack energy capacity 157 is 72.5 kWh, the pack weight is 630 kg, and the cycle life is 2000 times or 10 years. The energy density of the 158 battery is 180 Wh/kg at the cell level and 115 Wh/kg at the pack level. Figure 2 shows the material compositions of 159 a 1 kWh LIB pack, including the cell materials and battery components. The cathode active material, NCM 622, 160 accounts for 26.7% of the total LIB mass. The anode active material, graphite, accounts for 15.3% of the total LIB 161 mass. The wrought aluminum used for the cathode electrode and enclosure represents 23.0% of the total LIB mass. 162 The copper used for the anode electrode and terminal represents 8.6% of the total LIB mass. The electrolytes, 163 including LiPF₆, Ethylene Carbonate (EC) and DMC, account for 18.5% of the total LIB mass. The polypropylene 164 used for the separator comprises 1.5% of the total LIB mass. The battery components, including steel, thermal 165 insulation, coolant electronic parts and wrought aluminum, account for 9.3% of the LIB mass. Detailed material 166 compositions of NCM 622 pack are presented in Table S 4 in the Supporting Information.

167 3.3.2 Production stage

168 The production stage of NCM 622 battery includes cell manufacturing, module and pack assembly. Cell 169 manufacturing consists of the mixing, coating and drying, vacuum drying and formation processes. The primary data 170 are based on a cell production capacity of nearly 30 GWh/yr. A process-based and attributional approach was used 171 to compile the inventory data.

172 In order to manufacture 1 kWh of cell, 72.0 MJ of electricity and 34.0 MJ of steam are consumed. The coating 173 and drying process (dry room) consumes 25.2 MJ (35%) of electricity and 17.0 MJ (50%) of steam for 174 dehumidification. Subsequently, the electrode vacuum drying process consumes 28.8 MJ (40%) of electricity and 175 17.0 MJ (50%) of steam. Then, the formation process consumes 10.8 MJ (15%) of electricity. In addition, the 176 mixing process and module and pack assembly process consumes 3.6 MJ (5%) of electricity, respectively. Energy 177 consumption for per kWh NCM 622 battery production are presented in Table S6 in the Supporting Information. 178 Therefore, considering the 4 MJ/kWh electricity required to fully charge the battery, it is estimated that the total 179 energy consumption of the LIB production is 110.0 MJ/kWh. The vacuum drying contributes the largest share 180 (42%) of the total energy demand, followed by the coating and drying process (38%). Formation accounts for 10% 181 of the total energy demand. While the contribution of mixing process and module and pack assembly process are 182 relatively lower than the other processes, accounting for 3%, respectively. Besides, 33.9 kg water is used in the 183 mixing process, and 20 g particulate matter is emitted during the 1 kWh cell manufacturing.

184 3.3.3 End-of-life stage

185 The current main recycling technology for waste LIB include physical dismantling (Saeki et al., 2004; Zhang et 186 al., 2007), pyrometallurgy (Bahat et al., 2007; Song et al., 2013) and hydrometallurgy (Chen et al., 2015; Nayaka et 187 al., 2016; Sun and Qiu, 2012). In hydrometallurgy the materials in LIBs are selectively dissolved by chemical 188 solvents and the metal elements are separated in the leachate. It could be used alone or in combination with 189 pyrometallurgy and does not require high equipment and processing cost (Nayaka et al., 2016). Under optimized 190 experimental conditions the recovery efficiency of 98.7% for Ni, 97.1% for Mn, 98.2% for Co and 81.0% for Li 191 could be attained (Chen et al., 2015). Due to the wide application of hydrometallurgical methods for recycling waste 192 LIBs in China and in order to simplify our model, it is assumed that used NCM 622 batteries are 100% collected and 193 recycled by hydrometallurgical methods to feed into NCM 622 production loop and thus avoid the production of

- 194 primary materials, such as steel, aluminum, polypropylene and copper. From the onsite investigations in two
- 195 Chinese large waste battery recycling corporations, including the one owned by the world's top three LIB supplier
- 196 (Xie et al., 2015), and the other one that is the world's leading waste battery and cobalt nickel tungsten rare metal
- 197 recycling corporation, the inventory data associated with the recycling of 1 kWh of waste LIBs are shown in Table
- 198 1. The primary data is based on a waste battery treatment capacity of 3,000t/yr.
- 199 Table 1 Inventory Data for the Recycling of 1 kWh Waste NCM 622 Lithium-Ion Power Battery

Category	Name	Value	Unit
Materials	Waste NCM battery	1.0	kwh
	H ₂ SO ₄ (98%)	9.6	kg
	HCl (30%)	0.3	kg
	NaOH (30%)	16.3	kg
	Na ₂ CO ₃	0.2	kg
	Ammonia (28%)	1.0	kg
	Extracting reagent P507	17.4	g
	Kerosene	42.5	g
	H ₂ O ₂	3.2	kg
	Industrial water	121.6	kg
	Li ₂ CO ₃	1.1	kg
Energy	Electricity	20.3	kWh
	Natural gas	1.2	m3
Emissions	Wastewater	86.9	kg
	Ammonia nitrogen	0.5	g
	CO ₂	0.6	kg
	SO ₂	0.01	kg
	Dust	3.1	kg
Recycled	Polypropylene	0.1	kg
Substances	Copper	0.7	kg
	Aluminum	1.8	kg
	Steel	0.1	kg
	NCM Precursor	2.1	kg

200 4 Results and Discussion

201 4.1 Life cycle assessment results

The LCA results for the six environmental impact categories are shown in Figure 3. The material preparation stage is the primary contributor to all of the six environmental impact categories, accounting for more than 95% of the total value, respectively. These impacts are mainly attributed to the production of the cathode active material

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205	(NCM 622), wrought aluminum and DMC. For POCP and HTP, the contribution from the material preparation stage
206	takes account of around 200%, largely due to the production of wrought aluminum. The contribution of the
207	production stage is relatively lower than the material preparation stage, accounting for 20.3% of the total GWP,
208	12.8% of the total PED and 9.2% of the total AP, 7.0% of the total POCP, around 2% of the total EP and HTP,
209	respectively. In the production stage, cell manufacturing is the main contributor (around 95%) for all six impact
210	categories due to the high energy consumption. For all six impact categories, the end-of-life stage contributions are
211	negative. Waste NCM 622 battery recycling in the end-of-life stage can reduce 0.03 kg C_2H_4 e (105.2%) of the life
212	cycle POCP and 41.6 kg 1,4-DB e (139.8%) of the life cycle HTP, mainly because of the recycling of waste wrought
213	aluminum. Besides, waste NCM 622 battery recycling could also reduce 30.9 kg CO ₂ e (33.0%) of the life cycle
214	GWP and 158.3 MJ (14.7%) of the life cycle PED, due to the reproducing of NCM 622. The life cycle assessment
215	results for per kg NCM 622 battery are shown in Table S 7 in the Supporting Information.
216	Table 2 presents the LCIA results of 10 types of impact categories by using the ReCiPe Midpoint (H) V1.11 /

217 World Recipe H RECIPE method. It is found that the results of GWP, AP, POCP, EP and HTP are similar to those

assessed by the CML-IA baseline V3.02 method.

Table 2 Life cycle assessment results for per kWh NCM 622 battery (ReCiPe Midpoint (H) V1.11/ World Recipe H)

Impact category	Unit	Material	Production	End-of-life	Total
Climate change (GWP)	kg CO ₂ eq	105.47	19.01	-30.91	93.57
Terrestrial acidification (AP)	kg SO ₂ eq	0.47	0.05	-0.03	0.49
Photochemical oxidant formation (POCP)	kg NMVOC	0.34	0.04	-0.09	0.29
Freshwater eutrophication (EP)	kg P eq	0.01	0.00	0.00	0.01
Marine eutrophication (EP)	kg N eq	0.13	0.00	-0.11	0.02
Human toxicity (HTP)	kg 1,4-DB eq	26.01	0.61	-14.09	12.53
Terrestrial ecotoxicity	kg 1,4-DB eq	0.03	0.00	-0.02	0.01
Freshwater ecotoxicity	kg 1,4-DB eq	21.43	0.00	-19.93	1.5
Particulate matter formation	kg PM10 eq	0.15	0.01	-0.01	0.15
Metal depletion	kg Fe eq	6.06	0.00	1.73	7.79
Fossil depletion	kg oil eq	24.67	3.12	-3.65	24.14

220 **4.2 Identification of significant environmental impacts**

Figure 4 presents the relative contributions in the material preparation stage of 1 kWh NCM 622 battery. For

the PED and GWP, the cathode active material (NCM 622) and wrought aluminum are the top two contributors,

together accounting for around 75% of the battery materials. 60% of the AP, more than 40% of the PED and GWP is

224 contributed by the NCM 622. Wrought aluminum is the most substantial contributor to the POCP and HTP,

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accounting for more than 60% and 70% of the battery materials, respectively. For the EP, however, the predominant contributor is the electrolytes DMC (73.3%), followed by NCM 622 (15.4%). Graphite contributes 10.8% for the PED, 6.9% for the GWP, 4.2% for the AP and less than 2% in the other three impact categories in the material preparation stage. For all the six impact categories, copper, LiPF₆ and electronic parts account for less than 4%, 7% and 7% of the battery materials, respectively.

Figure 5 shows the relative contributions in the production stage of 1 kWh NCM 622 battery. Vacuum drying

231 process accounts for the largest proportion (more than 40%) for all the six environmental impact categories,

followed by the coating and drying (around 36%), due to the large share of the energy demand in these two

233 processes. Formation contributes to 10%~15% for the six environmental impact categories. The mixing process and

234 module and pack assembly process account for less than 5% for the six environmental impact categories,

235 respectively.

236 4.3 Comparative analysis

237 We compare the GHG emissions of NCM battery production (material preparation and production) with 238 existing literature studies in Figure 6. The total GHG emissions are disaggregated and associated with cell materials, 239 battery components, cell manufacturing, module and pack assembly and others. Figure 6 reports great variation in 240 the overall production GHG emissions with results ranging between 73 and 200 kg CO₂ e/kWh, showing different 241 contributions from cell materials, battery components, cell manufacturing and module and pack assembly. The result 242 for NCM battery production GHG emissions in this study is 124.5 kg CO₂ e/kWh, which is similar to that reported 243 by USEPA (2013). The production GHG emissions determined by MajeauBettez et al. (2011) where inventory data 244 from Ecoinvent 2.2 database were used are nearly two times higher than this study. They based their energy data on 245 industry reports published nearly 15 years ago, at their early commercialization stage, therefore it might not reflect 246 current NCM battery production practices (Dai et al., 2019; Rydh and Sandén, 2005). It seems that Ellingsen et al. 247 (2014) and Kim et al. (2016) where inventory data from Ecoinvent 3.1 database were used overestimated the energy 248 consumption during the cell manufacturing process, which are more than three times higher than those in this study. 249 The GHG emissions of the plant in the study of Ellingsen et al. (2014) and the underutilization of the plant in the 250 study of Kim et al. (2016) would lead to the overestimation of energy intensity for cell production (Dai et al., 2019). 251 The GHG emissions for cell manufacturing of this study (NCM 622) is similar with those of the study of Dai et al.

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(2019) (NCM 111), because the energy consumption data of this process are both based on Chinese factories. The
GHG emissions for cell materials of this study is much higher than Dai et al. (2019) where inventory data were also
supplemented by GREET model, as our study is for NCM 622 which represents the state-of-art technology in China,
while Dai et al. (2019) analyzed NCM 111 which represents the old-fashioned technology in China. The proportion
of GHG emissions in the module and pack assembly is less than 1% for all the studies except MajeauBettez et al.
(2011) (3%).

258 4.4 Sensitivity analysis

259 As shown in the section 4.1, the material preparation stage is the primary contributor to all the six 260 environmental impact categories, especially for the cathode active material, NCM622. The current trend of NCM 261 battery technology is to replace NMC622 by NMC811. Therefore, the sensitivity analysis is performed to evaluate 262 the impacts of replacing NMC622 by NMC811. Based on expert consultation, the mass of cathode active material 263 and battery energy density of the LIB are assumed to be not change despite the changes of the cathode active 264 material chemistry. The sensitivity analysis results show that the total life cycle GWP, AP and POCP could be 265 increased by around 1%, while the total life cycle PED, EP and HTP could be increased slightly by less than 0.3%. 266 This is primarily because the increased content of NiSO₄ in the production of NCM 811 Precursor results in 267 increased consumptions of steam, LiOH and oxygen for the final production of NCM 811 relative to per kg of NCM 268 622 (see Table S 2 and S 3 in the Supporting Information).

269 5 Conclusions

270 In this study, the environmental impacts of the most commonly used NCM 622 battery for passenger BEVs in 271 China were assessed throughout the life cycle. Primary data were collected from two Chinese leading LIB suppliers 272 (world's top three), two leading cathode material producer (world's top five), and two battery recycling corporations 273 (one is owned by the world's top three LIB supplier, and the other one is the world's leading waste battery and 274 cobalt nickel tungsten rare metal recycling corporation) from 2017 to 2019. The evaluation is presented in terms of 275 six impact categories following the CML-IA baseline V3.02 method: primary energy demand (PED), global 276 warming potential (GWP), acidification potential (AP), photochemical oxidant creation potential (POCP), 277 eutrophication potential (EP), and human toxicity potential (HTP). The study results can be listed as follows.

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278 Firstly, the material preparation stage is the largest contributor to all the six environmental impact categories, 279 largely due to the production of the cathode active material (NCM 622), wrought aluminum and electrolytes. The 280 contribution of the production stage is relatively lower than the material preparation stage. Waste LIB recycling in 281 the end-of-life stage could largely reduce the life cycle POCP and HTP of LIB, mainly because of the recycling of 282 waste wrought aluminum. Secondly, in the material preparation stage, the battery cell materials, including the 283 cathode active material and wrought aluminum are the predominant contributors to the PED and GWP. Wrought 284 aluminum is the most substantial contributor to the POCP and HTP, while the electrolytes are the predominant 285 contributor to the EP. Besides, electronic makes a considerable contribution to the HTP. In the production stage, 286 vacuum drying and coating and drying processes are the top two contributors. Finally, from the sensitivity analysis, 287 replacing NMC622 by NMC811 as the cathode active material could increase all the six environmental impacts. 288 However, the use stage is not included in the NCM 622 battery's system boundaries due to the large uncertainty 289 of some key parameters, such as the real world driving cycles, different charging behaviors, battery replacement 290 times, and the lack of unified allocation method of the electricity consumption of the battery pack. Therefore, when 291 considering the whole LIB life cycle, it could cause quite different results for different impacts when including the 292 use stage which shall be evaluated in the future studies when the key information is available. In order to better 293 perform LIB eco-design, future LIB technologies should also emphasize by optimizing of the cathode active 294 material with the preference on the impacts of different life cycle stages.

In addition, with the progress of LIB technology, continued environmental LCA efforts combined with the cost analysis based on primary data, especially for the recycling stage, are necessary to provide efficient strategies for full life cycle environmental impact reduction in LIBs and the whole value chain in sustainable development of BEVs.

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305 **Conflicts of interest**

- 306 None.
- 307

308

309 Nomenclature

Nomenclature		
Name	Abbreviation	
Acidification potential	AP	
Battery electric vehicles	BEVs	
China automotive life cycle database	CALCD	
Dimethyl carbonate	DMC	
Ethylene carbonate	EC	
Eutrophication potential	EP	
Fuel cell electric vehicles	FCVs	
Global warming potential	GWP	
Human toxicity potential	НТР	
Life cycle assessment	LCA	
Life cycle inventory	LCI	
Lithium iron phosphate	LiFePO ₄ , LFP	
Lithium manganese oxide	LiMn ₂ O ₄ , LMO	
Lithium nickel cobalt manganese oxide	LiNi _x Co _y Mn _z O ₂ , NCM	
Lithium-ion power batteries	LIBs	
Lithium-ion power battery	LIB	
New energy vehicles	NEVs	
Photochemical oxidant creation potential	POCP	
Plug-in hybrid electric vehicles	PHEVs	
Polyvinylidene fluoride	PVDF	
Primary energy demand	PED	

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- 385 Figure captions
- 386 Figure 1 System boundaries of NCM 622 batteries excluding use phase
- 387 Figure 2 Material compositions of per kWh NCM 622 battery
- 388 Figure 3 Life cycle assessment results for per kWh NCM 622 battery (CML-IA baseline V3.02)
- 389 Figure 4 Relative contributions of per kWh NCM 622 battery material
- 390 Figure 5 Relative contributions of per kWh NCM 622 battery production
- 391 Figure 6 GHG emissions of per kWh NCM battery production



Input material, energy flows

392

Output to air, water and land

393 Figure 1 System boundaries of NCM 622 batteries excluding use phase



395

396 Figure 2 Material compositions of per kWh NCM 622 battery. The material masses per kWh is calculated by (pack

397 energy density \times the material mass percentage of the pack) $\times 1/1000$





Figure 3 Life cycle assessment results for per kWh NCM 622 battery (CML-IA baseline V3.02)



- 405 Figure 4 Relative contributions of per kWh NCM 622 battery material



408 Figure 5 Relative contributions of per kWh NCM 622 battery production

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410

411 Figure 6 GHG emissions of per kWh NCM battery production

out

1 Supporting Information

2 Life cycle assessment of lithium nickel cobalt manganese oxide

3 (NCM) batteries for electric passenger vehicles

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- 13

15	As shown in Table S1, LCI data of metals (copper, wrought aluminum, steel and graphite), plastic
16	(polypropylene), electrolytes (LiPF $_6$ and ethylene carbonate (EC)), coolant, energy and resources
17	(electricity, steam, natural gas and water) were acquired from China Automotive Life Cycle Database
18	(CALCD).
19	CALCD represents the Chinese automotive industry and includes more than 20,000 unit

20 processes, such as basic processes and product data (transportation and waste treatment as well as

21 metals, minerals, plastics, water, chemicals, fuels, energy production, etc.) and life cycle data of auto

22 parts, conventional vehicles and NEVs.

23 Table S 1 Data Source List

parts, conventional vehicles and	NEVs.
Table S 1 Data Source List	
Name	Data source
Material	
NCM Precursor	Factory survey
Active Material: NCM	Factory survey
Graphite	Factory survey
Binder: PVDF	GREET 2018, CALCD 2018
Copper	CALCD 2018
Wrought Aluminum	CALCD 2018
Electrolyte: LiPF ₆	CALCD 2018
Electrolyte: EC	CALCD 2018
Electrolyte: DMC	GREET 2018, CALCD 2018
Plastic: Polypropylene	CALCD 2018
Steel	CALCD 2018
Thermal Insulation	CALCD 2018
Coolant: Glycol	CALCD 2018
Electronic Parts	GREET 2018, CALCD 2018
Energy and resources	
Electricity	CALCD 2018
Steam	CALCD 2018
Natural gas	CALCD 2018
Water	CALCD 2018

	Unit	NCM622	NCM811	Data source
Material inputs				
NiSO ₄	kg	1.0	1.3	Factory survey
$CoSO_4$	kg	0.3	0.2	GREET 2018, CALCD 2018
MnSO ₄	kg	0.3	0.2	Factory survey
NaOH (100%)	kg	0.9	0.9	Ecoinvent 3.0
NH ₄ OH (100%)	kg	0.1	0.1	Ecoinvent 3.0
Energy consumption				
Natural gas	m ³	1.1	1.1	CALCD 2018
Water consumption				
Water	m ³	0.6	0.6	CALCD 2018

24 Table S 2 Materials and Energy Flows for per kg NCM Precursor Production

25

26 Table S 3 Materials and Energy Flows for per kg NCM Production

	Unit	NCM622	NCM811	Data source
Material inputs				
Precursor	kg	1.0	1.0	Factory survey
Li ₂ CO ₃	kg	0.4		Ecoinvent 3.0
LiOH	kg		0.4	
Oxygen	m ³	3.0	3.2	Ecoinvent 3.0
Energy consumption				
Electricity	MJ	36.0	36.0	CALCD 2018
Steam	MJ	6.8	11.9	CALCD 2018
Water consumption				
Water	m ³	0.0003	0.0009	CALCD 2018

27

28

	Unit	Li ₂ CO ₃	LiOH	LiPF ₆
Inputs				
Calcite	kg	0.9	3.3	10.7
Coal	kg	0.6	1.2	8.1
Fluorspar	g	0.0	0.0	148.2
Gravel	kg	2.2	3.5	7.5
Crude oil	kg	0.3	0.6	1.8
Sodium chloride	kg	0.9	1.4	1.6
Carbon dioxide	g	85.5	151.8	901.6
Fluorine	g	0.0	0.0	342.9
Iron	g	37.4	72.5	301.0
Phosphorus	g	0.1	0.2	1369.3
Emission to air				
Carbon dioxide	kg	0.2	1.0	23.6
Carbon monoxide	g	5.1	14.6	137.7
Phosphorus trichloride	g	0.0	0.0	348.3
Sulfur dioxide	g	10.0	21.2	241.1
Sulfate	g	10.5	19.9	123.0
Emission to water				
Calcium	g	62.0	131.8	35.0
Chloride	g	159.8	245.8	229.8
Magnesium	g	0.2	0.5	3.0
Silicon	g	4.0	8.7	38.5
Sodium	g	10.5	19.9	123.0
Suspended solids	g	6.5	16.4	123.7

30 Table S 4 Life Cycle Inventory for per kg Li_2CO_3 , LiOH and LiPF₆ Production

32	Table S 5 BOM of the	reference 72.5	kWh NCM622	battery pack
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Material name	Mass (kg)	Percentage	Material type
Active Material: NCM622	168.3	26.7%	Cell materials
Graphite	96.2	15.3%	Cell materials
Binder:Polyvinylidene Fluoride (PVDF)	12.0	1.9%	Cell materials
Copper	54.1	8.6%	Cell materials
Wrought Aluminum	145.1	23.0%	18.1% for cell materials, 4.9%
			for battery components
Electrolyte: LiPF ₆	7.2	1.1%	Cell materials
Electrolyte: Ethylene Carbonate	75.2	11.9%	Cell materials
Electrolyte: Dimethyl Carbonate	34.3	5.4%	Cell materials
Plastic: Polypropylene	9.6	1.5%	Cell materials
Steel	6.3	1.0%	Battery components
Thermal Insulation	1.9	0.3%	Battery components
Coolant: Glycol	10.1	1.6%	Battery components
Electronic Parts	9.5	1.5%	Battery components

33 Table S 6 Energy consumption for per kWh NCM 622 battery production

	Cell manufacturing						
	Mixing	Coating and	Vacuum	Formation	assembly	Total	
	WIIXINg	drying	drying	1 of mation	ussemerj		
Electricity (MJ/kWh)	3.6	25.2	28.8	10.8	3.6	72.0	
Steam (MJ/kWh)		17.0	17.0			34.0	
Water (kg/kWh)	33.9					33.9	

34

35

36 Table S 7 Life cycle assessment results for per kg NCM 622 battery

Impact category	Raw material	Production	End-of-life	Total
PED (MJ)	118.3396	9.5002	-11.0553	116.7845

	Journal Pre-proof					
GWP (kg CO ₂ e)	11.4301	1.9852	-2.9232	10.4920		
AP (kg SO ₂ e)	0.0539	0.0053	0.0019	0.0610		
POCP (kg $C_2H_4 e$)	0.0055	0.0002	-0.0029	0.0028		
$EP (kg PO_4^{3-} e)$	0.0311	0.0006	0.0031	0.0348		
HTP (kg 1,4-DB e)	9.6152	0.0473	-3.8837	5.7788		

37 Table S 8 Life cycle assessment results for per kg Li₂CO₃, LiOH and LiPF₆ Production

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Impact category	Li ₂ CO ₃	LiOH	LiPF ₆
PED (MJ)	33.5528	71.4924	317.4423
GWP (kg CO ₂ e)	2.6085	6.2171	29.2780
AP (kg SO ₂ e)	0.0203	0.0401	0.3417
POCP (kg $C_2H_4 e$)	0.0007	0.0017	0.0164
$EP (kg PO_4^{3-} e)$	0.0032	0.0066	0.0286
HTP (kg 1,4-DB e)	0.7016	1.5142	29.6353

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Conflicts of interest

The authors declare no conflicts of interest.

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