

# Classification of cathode materials for lithium-ion batteries of new energy electric vehicles based on safety and dynamic performance

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**Abstract.** The severe environmental pollution caused by fossil fuels has driven the demand for new energy vehicles. The choice of cathode materials for lithium-ion batteries is a major difficulty to be overcome in the development of new energy vehicles. Based on the performance characteristics of new energy vehicle batteries in actual use, this paper classifies the six most widely used cathode electrode materials in the new energy vehicle market. Firstly, the temperature data of power batteries with different cathode materials in the overcharge experiment and acupuncture experiment were collected to characterize the safety performance of power batteries. Then the maximum specific discharge capacity and operating voltage data of the battery were collected, and the maximum specific discharge energy of the battery was calculated to study the dynamic performance of the vehicle. After that, the safety performance and dynamic performance of each index is compared. Finally, according to the safety performance and dynamic performance of the corresponding power battery, the six cathode materials are divided into three types: power type, safety type, and balanced type. According to the classification results, it can be concluded that the design of balanced cathode materials with both safety and dynamic performance is the best development route for future new energy vehicle batteries.

**Keywords:** New energy vehicle, Lithium-ion battery, Cathode materials

## 1. Introduction

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With the annual growth rate of more than 30 million vehicles worldwide [1], motor fuels such as diesel and gasoline have become one of the main causes of the greenhouse effect and global warming. Following the concept of green energy and low-carbon economy put forward in the Paris Agreement, various countries have introduced relevant policies for low-carbon emission reduction [2]. New energy vehicles are gradually replacing fuel vehicles under the promotion of policies. New energy vehicles are

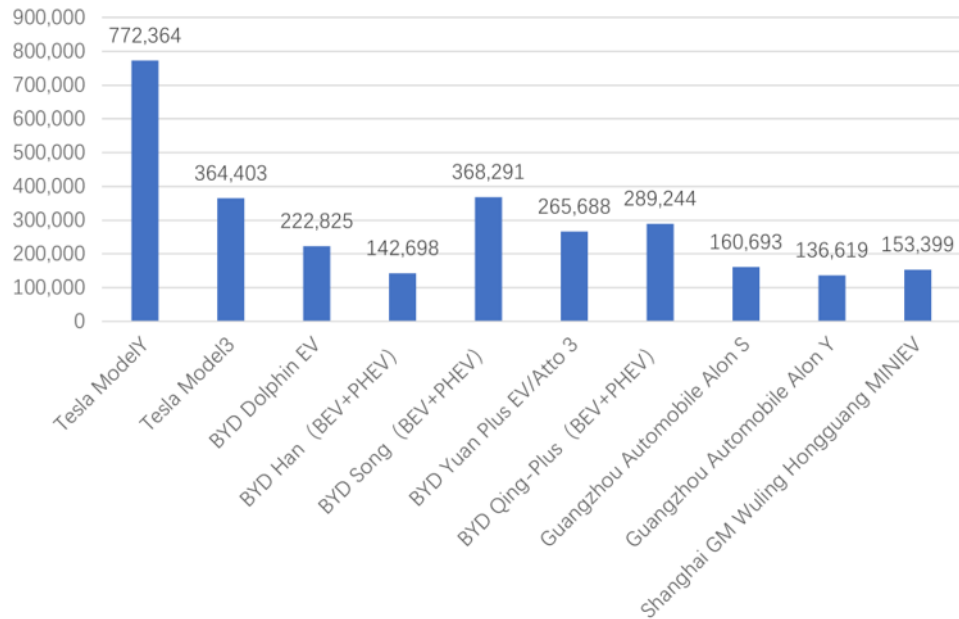
gradually replacing fuel vehicles under the promotion of policy. New energy vehicles take electric energy as the main energy source, and their technical core and manufacturing difficulty are mainly concentrated on power battery technology [3]. At present, the most common new energy vehicle power batteries are lead-acid batteries, nickel-hydrogen batteries, lithium-ion batteries, and fuel cells, of which lithium-ion batteries are regarded as the development direction of future power batteries [4]. In the components of lithium-ion batteries, the choice of battery cathode materials plays a role in affecting the safety and dynamic performance of lithium-ion batteries. Therefore, it is of great significance to study the performance characteristics of lithium-ion battery cathode materials for the development of the entire new energy automobile industry.

In the existing classification of different types of cathode materials for lithium-ion batteries, An Fuqiang et al. [5] divided lithium-ion batteries into first-generation batteries represented by lithium cobalt oxide, second-generation batteries represented by lithium iron phosphate and third-generation batteries dominated by ternary batteries according to the development sequence of cathode material. Li Wei et al. [6] divided lithium-ion batteries into one-yuan batteries including lithium cobaltate and lithium nickelate, binary batteries including lithium nickel cobaltate and ternary batteries represented by nickel-cobaltate-manganese ternary oxides according to different combinations of nickel, cobalt, and manganese in the cathode materials. Yan Jinding [7] and Ming Bo et al. [8] classified lithium-ion batteries into hexagonal layered structure material batteries represented by lithium cobaltate and lithium nickelate, spinel structure material batteries represented by lithium manganate, and olivine structure material batteries represented by lithium iron phosphate according to the different micro-spatial structures of cathode materials. Wang Pengbo et al. [9] classified them into layered oxide batteries, multiple composite oxide batteries, spinel-type oxide batteries, polyanionic compound batteries, and lithium-rich materials batteries according to the crystal structure of the cathode component materials. It can be seen that the classification of lithium-ion cathode materials mainly focuses on the physical or chemical properties of independent cathode materials. At present, there is almost no research on the classification of cathode electrode materials in accordance with the actual use characteristics of new energy vehicle batteries.

Based on the lack of classification of cathode materials according to actual use characteristics, this paper focuses on new energy vehicles with high sales volume and the use of unique cathode materials in the current market. Taking the six most widely used cathode materials as the research object, the corresponding six lithium-ion batteries are classified according to power batteries' safety and dynamic performance characteristics. This classification will determine the three development paths of existing new energy vehicle cathode materials, and looks forward to the best development direction of the future new energy vehicle cathode materials industry.

## **2. Cathode materials**

The "Global New Energy Passenger Vehicle Sales Data" [10] released by CleanTechnica statistics the top 20 models of global new energy vehicle sales from January to August 2023. Among them, the brand, model, and sales data of the top ten vehicles are shown in Figure 1, and the cathode materials of electric batteries used are shown in Table 1. On this basis, a small number of other new energy passenger vehicles that also use lithium-ion batteries but have unique cathode materials are selected as supplements. Their brands, models, and cathode materials of electric batteries are shown in Table 2.



**Figure 1.** Data of the top ten global new energy passenger vehicle sales from January to August 2023 (Unit: vehicles)

**Table 1.** Top 10 electric vehicle cathode materials in global new energy passenger vehicle sales from January to August 2023

Automobile Brand	Vehicle Model	Cathode Material
Tesla	Model Y	NCM523 [11]
	Model 3	LFP [12]
BYD	BYD Dolphin EV	LFP [13]
	Han (BEV+PHEV)	LFP
	Song (BEV+PHEV)	LFP
	Yuan Plus EV/Atto 3	LFP
	Qing-Plus (BEV+PHEV)	LFP
Guangzhou Automobile	Alon S	NCM811 [14]
	Alon Y	LFP [15]
Shanghai GM Wuling	Hongguang MINIEV	LFP/NCM [16]

**Table 2.** New energy passenger car brand models and cathode materials for electric batteries as supplementary

Automobile Brand	Vehicle Model	Cathode Material
Nissan	Leaf	LMO&LCO [17]
Tesla	Model S	NCA [18]
	Roadster	LCO [19]
BYD	Qing-Pro EV	NCM523 [20]
Ford Motor	Mustang Mach-E	NCM811 [21, 22]
Audi	e-tron	NCM523 [23]

According to the statistics of cathode materials used by the top ten new energy passenger vehicles and supplementary models in 2023 in Tables 1 and Table 2, a summary can be obtained that the power batteries of new energy passenger vehicles on the market mainly use six cathode materials, including NCM523, NCA, NCM811, LFP, LCO, and LMO.

### 3. Power battery performance evaluation

#### 3.1. Safety performance

According to the “China New Energy Vehicle Safety Development Report” [24] released in March 2023, there were more than 3000 fire accidents of new energy electric vehicles in China in 2021, which was 1.5-3 times higher than the annual fire accident rate of traditional fuel vehicles. Among them, more than 50% of the causes of fire accidents are directly or indirectly related to the battery, and the spontaneous combustion of power batteries has become the main factor endangering the life safety of people in the car. The spontaneous combustion of batteries is also known as thermal runaway [25]. The occurrence of thermal runaway is usually related to the internal short circuit of batteries, improper charging, and external short circuit of batteries [26]. In the study of the thermal runaway of power batteries, the overcharge method [27] and acupuncture method [28] are usually used to simulate the extreme conditions of external use, to realize the inspection of the safety performance of electric batteries.

*3.1.1. Overcharge experiment.* During the use of new energy electric vehicles, overcharging will accelerate the aging process of the battery, attenuate the battery capacity, and increase the inconsistency between the battery units [29]. Overcharging for a long time will cause the rise of the temperature of the battery and the safety risks [30]. The safety of the power battery can be evaluated by collecting data of the highest temperature that the battery shell can reach when the six kinds of power batteries are overcharged at a constant charging rate. The corresponding experimental charging rates of the six power batteries and the maximum temperature of the battery housing are shown in Table 3.

**Table 3.** The charging rate and the maximum temperature of the battery shell in the overcharge experiment of six power batteries

Cathode Material	Charging Rate (Unit: C)	Maximum temperature of the battery shell (Unit: °C)
NCM523	1	891 [31]
NCA	1	635 [32]
NCM811	0.5	644.98
LFP	1	300
LCO	1	550 [33]
LMO	3	290 [34]

Table 3 shows that the maximum battery housing temperature that can be achieved by overcharging NCM523 is significantly higher than that of other kinds of batteries at the 1C charging rate. When the 3C charging rate of LMO is significantly higher than that of other types of batteries, the maximum temperature of the battery shell can reach 290°C, which is much lower than that of other types of batteries with lower charging rates. This result indicates that the safety of the NCM523 battery is poor in the overcharge state, and the safety of the LMO is better in the overcharge state.

*3.1.2. Acupuncture experiment.* In the driving process of new energy electric vehicles, sudden situations such as foreign bodies on the road and driving accidents may cause the battery pack to be punctured by external objects, cause an internal short circuit of the battery, and even spontaneous combustion of the battery, which threatens the safety of passengers. Acupuncture experiments can simulate such

emergencies and reflect the thermal runaway and safety performance of the power battery. A power battery with full charge (SOC=100%) is used in this experiment. A 3-8mm diameter high-temperature resistant tungsten needle is used to run vertically through the geometric center of the battery plate to detect the maximum temperature and average heating rate that can be achieved by the battery shell. Table 4 shows the highest temperature and average heating rate of the battery shell of the six kinds of power cells under the acupuncture experiment.

**Table 4.** The maximum temperature and average heating rate of the battery shell in the acupuncture experiment of six power batteries

Cathode Material	Maximum temperature of the battery shell (Unit: °C)	The average heating rate of the battery shell (Unit: °C/s)
NCM523	352.4	15.6
NCA	-	-
NCM811	542 [35]	4.3
LFP	306.7	80.2
LCO	-	-
LMO	111	1.85

Note: “-” means that the relevant test data is not found.

According to Table 4, it can be concluded that the maximum temperature of the NCM811 shell under the acupuncture experiment is significantly higher than that of other kinds of power batteries, while it has a slower heating rate. LFP shell has the fastest heating rate, but the highest temperature that can be reached is relatively low. The highest temperature the LMO battery can reach under the acupuncture test is 111°C, which is far lower than other kinds of power batteries. It has the slowest heating rate of 1.85°C/s and is the safest of all the batteries.

### 3.2. Dynamic performance

Among all the power battery parameters to evaluate the performance of new energy electric vehicles, the theoretical specific capacity, the maximum discharge specific capacity of the battery under constant conditions, and the operating voltage of the battery are directly determined by the type of cathode material. The theoretical specific capacity of the power battery refers to the maximum amount of electricity that can be provided when all the active substances in the lithium-ion battery per unit mass participate in the battery reaction under the ideal state. It can be calculated from the electrode reaction equation. The maximum specific discharge capacity of the battery under constant conditions is related to the manufacturing process of the battery, which represents the maximum amount of power battery per unit mass that can be released when the battery capacity is not attenuated during actual use. The operating voltage reflects the discharge ability of the power battery, and its product with the maximum discharge specific capacity is the maximum discharge specific energy. The maximum discharge specific energy refers to the maximum energy that can be released by the power battery per unit mass in actual use, which directly reflects the endurance of the power vehicle.

Comparing new energy electric vehicles carrying the same mass but different types of power batteries, the result of the product of the maximum specific discharge capacity of the battery and the working voltage is the maximum specific discharge energy. The larger the maximum specific discharge energy, the more energy the battery can release in a given time. The corresponding new energy vehicles will have a longer driving distance and better endurance.

**Table 5.** The theoretical specific capacity, maximum discharge specific capacity, operating voltage, and maximum discharge specific energy of six kinds of power batteries

Cathode Material	Theoretical Specific Capacity (Unit: mAh/g)	Maximum Specific Discharge Capacity (Unit: mAh/g)	Operating Voltage (Unit: V)	Maximum Specific Discharge Energy (Unit: mWh/g)
NCM523	278	207 [36]	4.3 [37]	890.1
NCA	279	196.5 [38]	4.3	844.95
NCM811	275	240 [39]	3.8	912
LFP	170	154 [40]	3.4	523.6
LCO	274	173.3 [41]	4.2 [42]	727.86
LMO	148	110 [43]	4.15	456.5

The corresponding theoretical specific capacity, the maximum discharge specific capacity under the condition of 0.1C, and the battery operating voltage parameters of the six power batteries are shown in Table 5. According to the data in Table 5, the theoretical specific capacity of NCM523, NCA, NCM811, and LCO is close to 280mAh/g, much higher than the other two kinds of batteries. This suggests that these four types of batteries have the greatest potential to store electricity. The actual maximum discharge specific capacity of NCM811 is much higher than that of other power batteries under the discharge condition of 0.1C, which is close to the theoretical specific capacity, but its operating voltage is lower. In general, the dynamic performance of NCM523, NCA, and NCM811 is better, and they all have maximum discharge specific energy of more than 800mAh/g. The theoretical specific capacity and maximum discharge specific energy of LMO are the lowest, and the endurance of electric vehicles is relatively lower than that of other types of electric vehicles.

#### 4. Classification

##### 4.1. Data treating

**Table 6.** Relative values of six power battery safety parameters

Cathode Material	The highest relative temperature of the battery housing in the acupuncture experiment (Unit: °C)	The relative value of the highest temperature of the battery shell in the overcharge experiment (Unit: °C)	The relative value of the average heating rate of the battery shell in the overcharge experiment (Unit: °C/s)	Total	Average
NCM523	0.33	0.31	0.12	0.76	0.25
NCA	0.46	-	-	0.46	0.46
NCM811	0.45	0.20	0.43	1.08	0.36
LFP	0.97	0.36	0.02	1.35	0.45
LCO	0.53	-		0.53	0.53
LMO	1.00	1.00	1.00	3.00	1.00

Note: Labeled “-” indicates no relevant experimental data, and only dividing by the known number of data was used in the calculation of the mean.

**4.1.1. Safety performance.** The LMO experimental data with the best safety performance in the overcharge and acupuncture experiments were used as the benchmark (marked yellow, and the relative value was denoted as “1”), and the three experimental data of LMO were divided by the corresponding data of the other five batteries. The relative values, the sum of the relative values, and the average relative values of the five power battery safety parameters are shown in Table 6.

**4.1.2. Dynamic performance.** According to the data in Table 5, NCM523 with the highest theoretical specific capacity and working voltage, and NCM811 with the highest maximum discharge specific capacity and maximum discharge specific energy were selected as the benchmark (marked in yellow, and the relative value was denoted as “1”).

**Table 7.** Relative values of dynamic performance parameters of six power batteries

Cathode Material	Relative theoretical specific capacity	Relative maximum discharge specific capacity	Relative value of operating voltage	Maximum relative specific energy	Total	Average
NCM523	1.00	0.86	1.00	0.98	3.83	0.96
NCA	1.00	0.82	1.00	0.93	3.75	0.94
NCM811	0.99	1.00	0.88	1.00	3.87	0.97
LFP	0.61	0.64	0.79	0.57	2.62	0.65
LCO	0.98	0.72	0.98	0.80	3.48	0.87
LMO	0.53	0.46	0.97	0.50	2.45	0.61

#### 4.2. Classification

Using the results obtained in Table 6, the safety performance of different cathode materials was classified with 0.45 and 0.8 as the dividing line. LMO batteries with an average relative value greater than 0.8 have excellent safety performance. The LCO, LFP, and NCA batteries with average relative values between 0.8 and 0.45 have good safety performance. The safety performance of NCM811 and NCM523 batteries with an average relative value of less than 0.45 is poor.

As for Table 7, 0.8 and 0.9 are used as the dividing line to divide the dynamic performance of different batteries. NCM523, NCA, and NCM811 batteries with an average relative value greater than 0.9 have excellent power performance. LCO with an average relative value between 0.8 and 0.9 have good dynamic performance, while LFP and LMO with an average relative value less than 0.8 have poor power performance.

**Table 8.** Classification of six power batteries

Cathode Material	Safety performance	Dynamic performance	Type
NCM523	Poor	Excellent	Power-type
NCA	Good	Excellent	Balanced-type
NCM811	Poor	Excellent	Power-type
LFP	Good	Poor	Safety-type
LCO	Good	Good	Balanced-type
LMO	Excellent	Poor	Safety-type

According to the classification of safety performance and dynamic performance of power batteries with different cathode materials, power batteries can be finally divided into three categories: (1) Power-type with poor safety performance but better dynamic performance; (2) Safety-type with good safety performance and above but poor dynamic performance; (3) Balanced-type with both good safety

performance and good dynamic performance. The classification results according to this principle are shown in Table 8.

As can be seen from Table 8, NCM523 and NCM811 batteries are power-type batteries, which have outstanding advantages in discharge specific capacity and discharge specific energy, corresponding to new energy vehicles that have good endurance. LFP and LMO batteries are safety-type batteries, which have lower heating rates and maximum temperature under the condition of thermal runaway and can better ensure the personal safety of passengers in accidents. NCA and LCO batteries are balanced type batteries, which can ensure a long driving time and cope with thermal runaway during driving.

## 5. Conclusion and outlook

Problems such as the greenhouse effect and global warming have accelerated the urgent demand for new energy vehicles, which has led to the research of lithium-ion battery cathode materials. According to the characteristics of safety performance and dynamic performance, six kinds of cathode materials that have been put into actual production can be divided into three types: dynamic type, safe type and balanced type. These three categories correspond to the three major development directions of existing lithium-ion power batteries: focusing on dynamic performance, focusing on safety performance, and focusing on both safety and dynamic balance development. Based on the expectation that new energy vehicles will fully replace existing fuel vehicles, it is clear that the development path that takes into account safety performance and power performance is the main choice for the development of lithium-ion batteries in the future.

However, by analyzing the performance test data of existing balanced anode materials (NCA, LCO) corresponding to lithium-ion batteries, it can be seen that it is difficult for balanced anode materials to have the best safety performance and dynamic performance at the same time. In terms of dynamic performance, the gap between the actual capacity and the theoretical capacity of LCO and NCA indicates that there is still room for improvement in the actual capacity of balanced cathode materials. In terms of safety performance, the lack of acupuncture experimental data has hindered a detailed analysis of the development trend of NCA and LCO. In this regard, other safety experiment data of NCA and LCO should be collected on the basis of existing research to conduct supplementary research on safety performance in the future.

The pursuit of the actual capacity of the battery and the consideration of the risk of thermal runaway of the battery make the cathode electrode materials used in lithium-ion power batteries difficult to unify. In this regard, researchers should first pay attention to the actual capacity and safety of existing cathode materials. In addition, composite cathode materials or new cathode materials with more potential and application prospects can be developed. On this basis, cost factors are added to lay the foundation for the comprehensive coverage of new energy vehicles and the realization of pollution-free travel in the future.

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