

## **Supporting information**

### **Selective recovery of valuable materials from bulk retired ternary lithium-ion batteries based on carbon monoxide reduction**

Zhen Xiong<sup>a,b,c</sup>, Hairong Zhang<sup>a,b,c\*</sup>, Haijun Guo<sup>a,b,c</sup> Mengkun Wang<sup>a,b,c</sup>, Can

Wang<sup>a,b,c</sup>, Hailong Li<sup>a,b,c</sup>, Xiong Lian<sup>a,b,c</sup>, Xuefang Chen<sup>a,b,c</sup>, Xinde Chen<sup>a,b,c\*</sup>

<sup>a</sup>School of Energy Science and Engineering, University of Science and Technology of China, Hefei 230026, PR China

<sup>b</sup>Guangzhou Institute of Energy Conversion, Chinese Academy of Sciences, No.2 Nengyuan Road, Tianhe District, Guangzhou 510640, PR China

<sup>c</sup> R&D Center of Xuyi Attapulgite Energy and Environmental Materials, Xuyi 211700, PR China

\* Corresponding author.

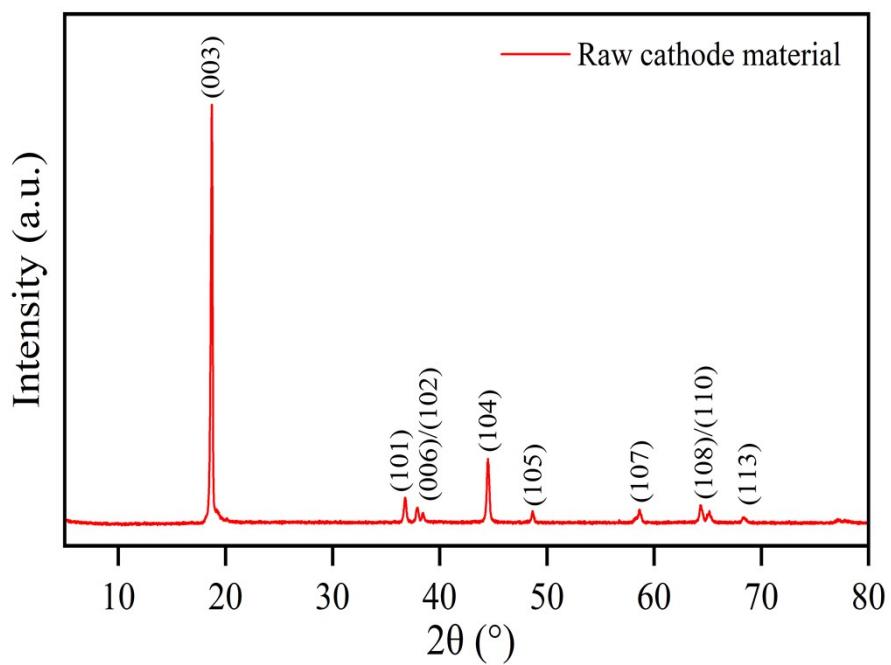
Address: No.2 Nengyuan Road, Tianhe District, Guangzhou 510640, China.

E-mail address: zhanghr@ms.giec.ac.cn (Hairong Zhang); Fax: +862037213916;  
Tel: +862087020234

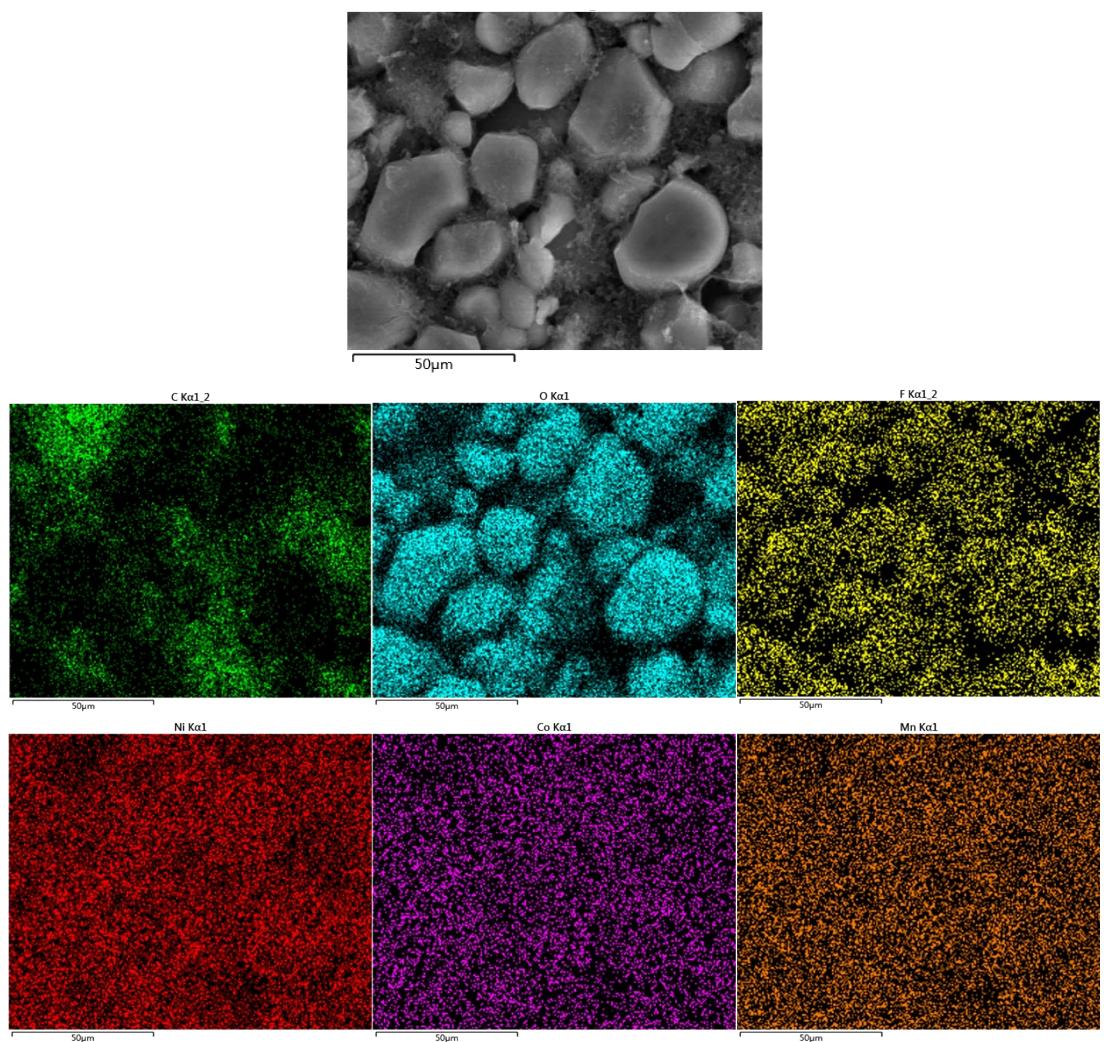
\*\* Corresponding author.

Address: No.2 Nengyuan Road, Tianhe District, Guangzhou 510640, China.

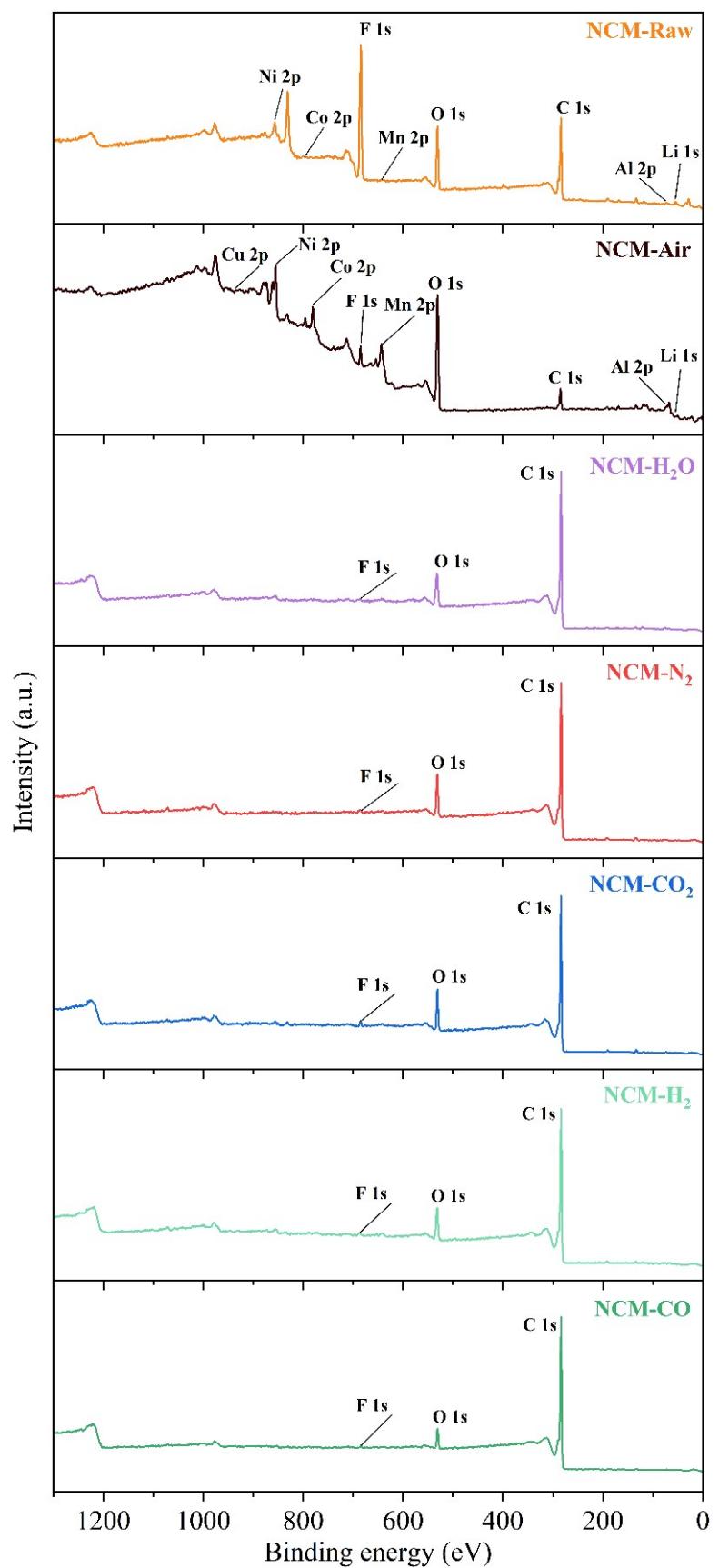
E-mail address: cxd\_cxd@hotmail.com (Xinde Chen); Fax: +862037213916;  
Tel: +862037213916



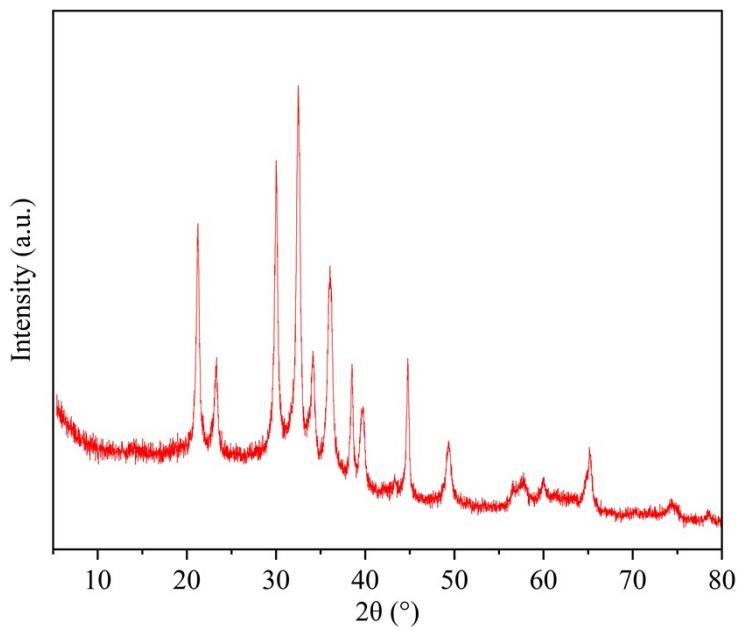
**Fig. S1** XRD pattern of the cathode material



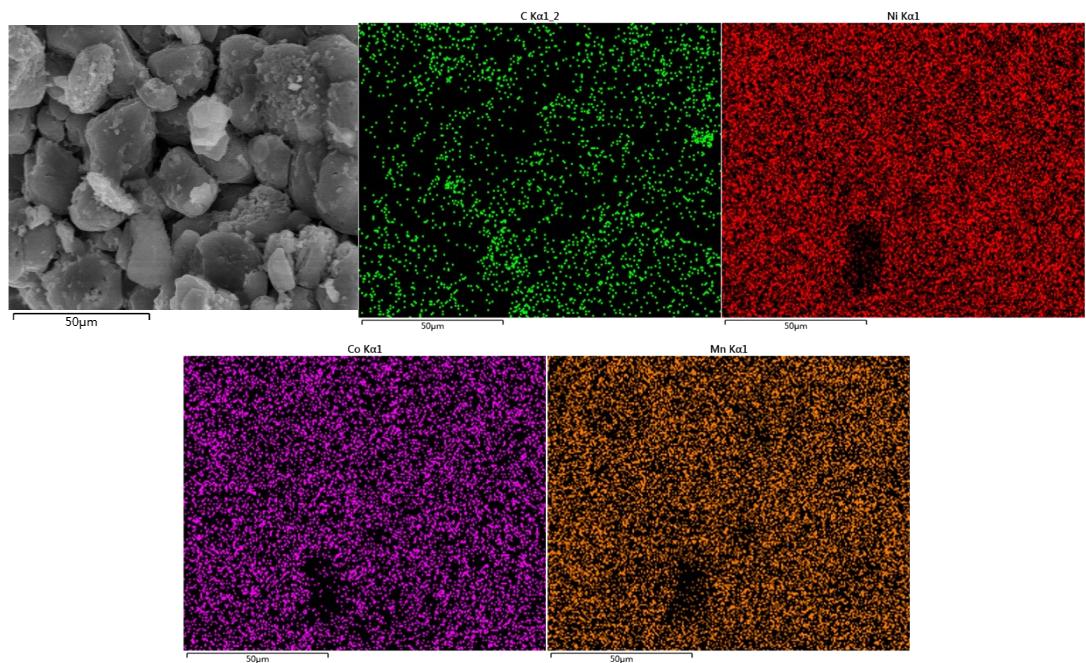
**Fig. S2** SEM images and EDS mapping of the spent cathode materials



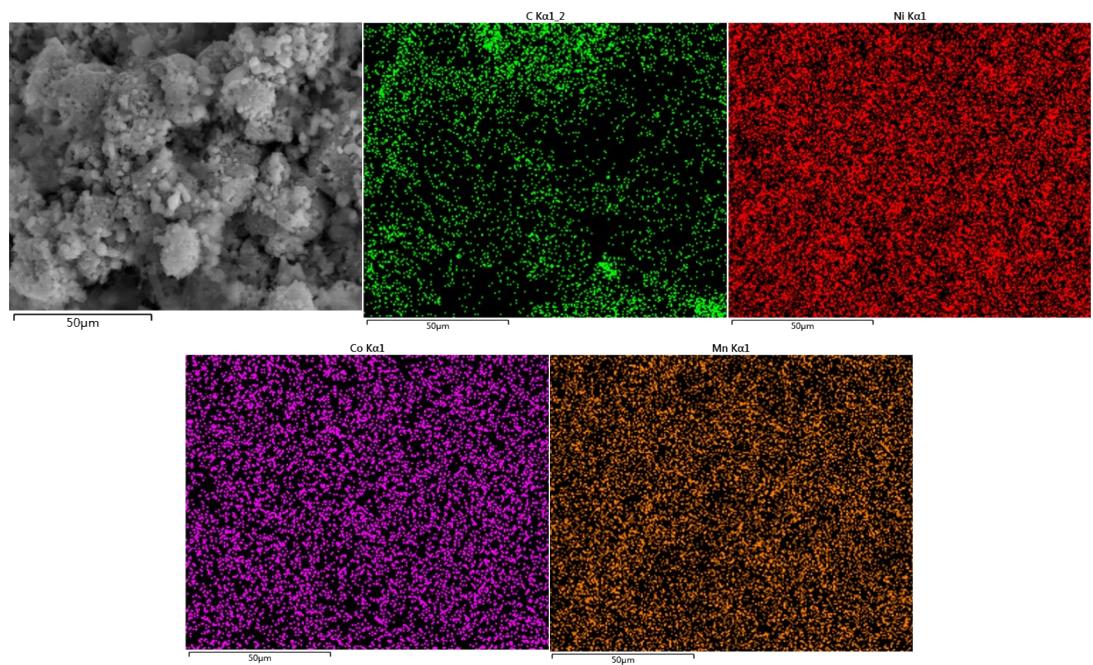
**Fig. S3** XPS spectra (broad scan) of roasting products under different atmosphere



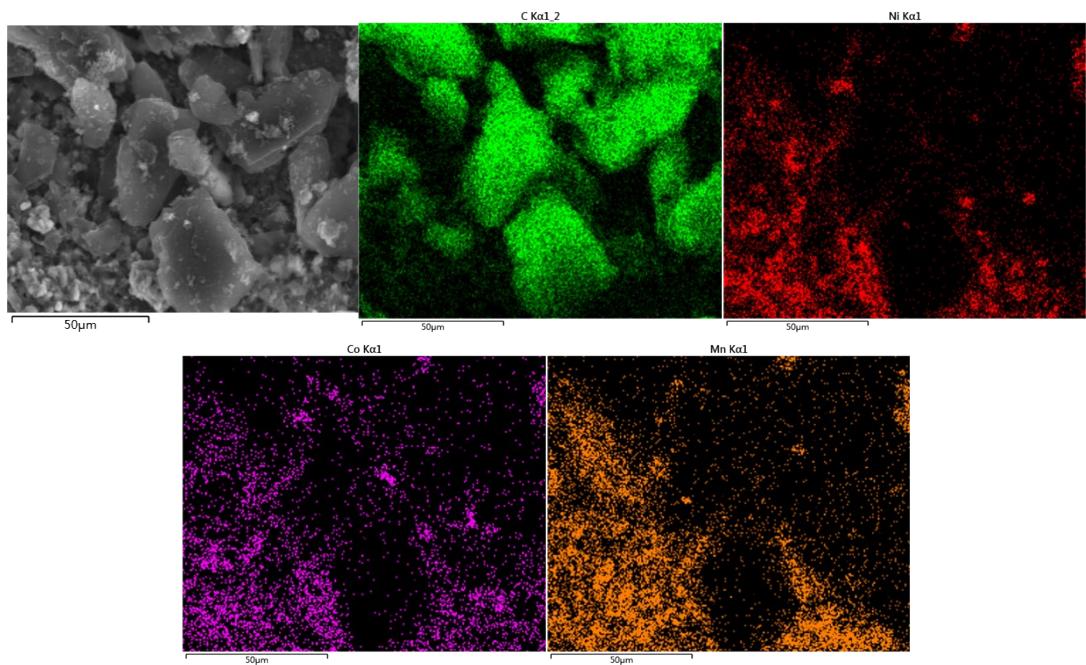
**Fig. S4** XRD patterns of the powder from water leaching solution



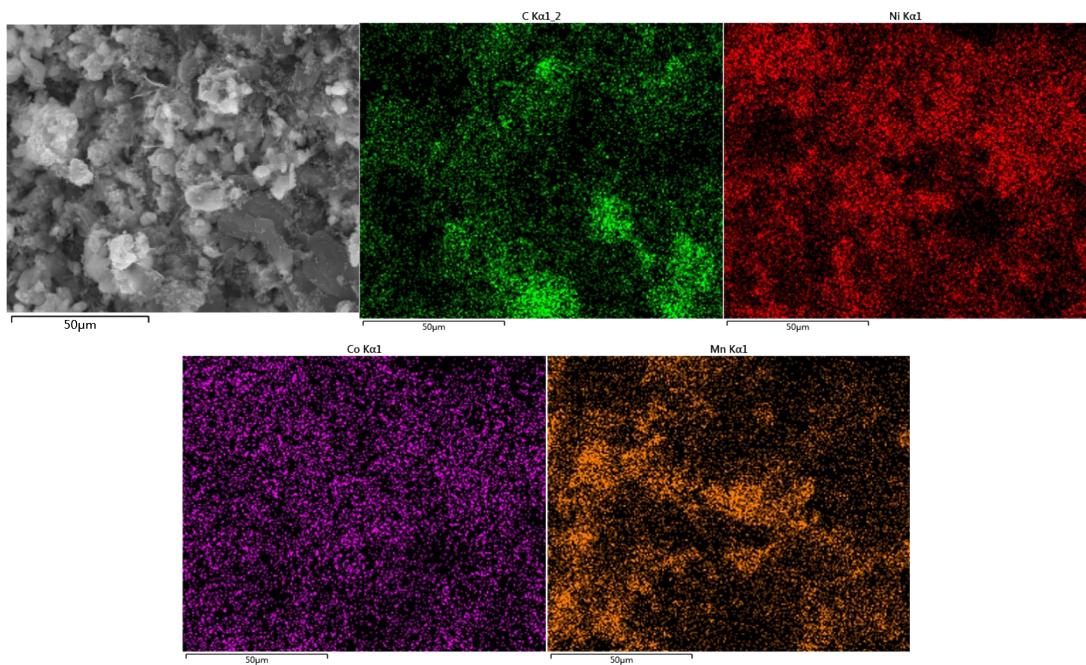
**Fig. S5** SEM images and EDS mapping of NCM-Air (650 °C, 6h)



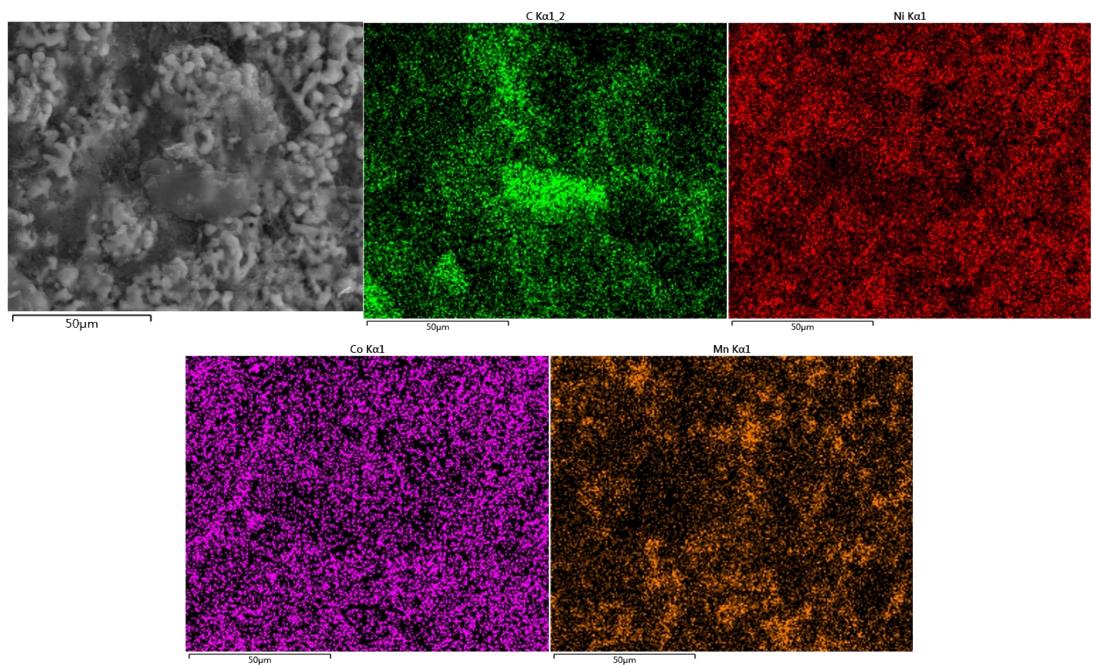
**Fig. S6** SEM images and EDS mapping of NCM-H<sub>2</sub>O (650 °C, 6h)



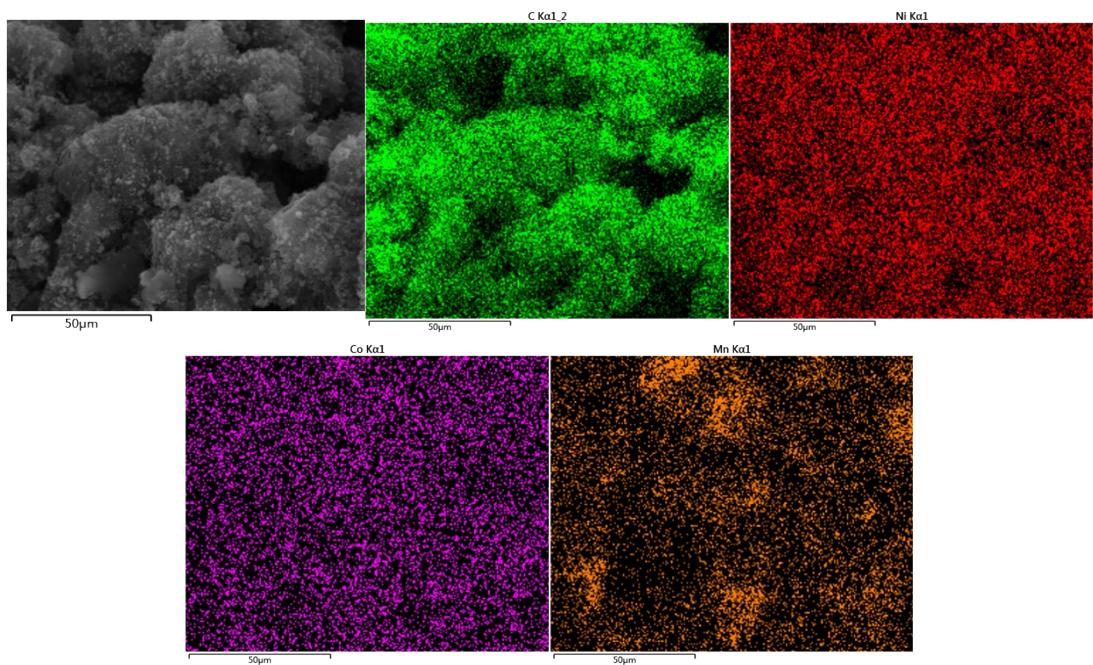
**Fig. S7** SEM images and EDS mapping of NCM-N<sub>2</sub> (650 °C, 6h)



**Fig. S8** SEM images and EDS mapping of NCM-CO<sub>2</sub> (650 °C, 6h)



**Fig. S9** SEM images and EDS mapping of NCM-H<sub>2</sub> (650 °C, 6h)



**Fig. S10** SEM images and EDS mapping of NCM-CO (650 °C, 6h)

**Table S1** Assignment analysis of Ni in the XPS spectra of raw material and roasting products. (650 °C, 6h)

| Sample               | Ni 2p <sub>3/2</sub> |                  |        |            |
|----------------------|----------------------|------------------|--------|------------|
|                      | Valence state        | Peak position/eV | At%    | References |
| NCM-Raw              | +3                   | 856.61           | 100.00 | 1-4        |
| NCM-Air              | +2                   | 854.30           | 42.19  | 3, 5-7     |
|                      | +3                   | 855.87           | 57.81  |            |
| NCM-H <sub>2</sub> O | 0                    | 852.52           | 13.76  | 8-10       |
|                      | +2                   | 854.57           | 86.24  |            |
| NCM-N <sub>2</sub>   | 0                    | 851.65           | 21.01  | 8-10       |
|                      | +2                   | 854.65           | 78.99  |            |
| NCM-CO <sub>2</sub>  | 0                    | 852.09           | 15.81  | 8-10       |
|                      | +2                   | 855.07           | 84.19  |            |
| NCM-H <sub>2</sub>   | 0                    | 851.89           | 13.24  | 8-10       |
|                      | +2                   | 854.62           | 86.76  |            |
| NCM-CO               | 0                    | 852.08           | 15.61  | 8-10       |
|                      | +2                   | 854.99           | 84.39  |            |

**Table S2** Assignment analysis of Co in the XPS spectra of raw material and roasting products. (650 °C, 6h)

| Sample               | Co 2p <sub>3/2</sub> |                  |       |                  |
|----------------------|----------------------|------------------|-------|------------------|
|                      | Valence state        | Peak position/eV | At%   | References       |
| NCM-Raw              | +2                   | 781.69           | 52.09 | 1, 3, 4, 11-13   |
|                      | +3                   | 780.19           | 47.91 |                  |
| NCM-Air              | +2                   | 782.11           | 32.49 | 1, 3, 11, 12, 14 |
|                      | +3                   | 780.35           | 67.51 |                  |
| NCM-H <sub>2</sub> O | 0                    | 778.54           | 14.70 |                  |
|                      | +2                   | 782.05           | 37.80 | 11, 15, 16       |
|                      | +3                   | 780.14           | 47.50 |                  |
| NCM-N <sub>2</sub>   | 0                    | 778.54           | 17.85 | 12, 15, 16       |
|                      | +2                   | 781.54           | 82.15 |                  |
| NCM-CO <sub>2</sub>  | 0                    | 778.76           | 20.45 | 12, 15, 16       |
|                      | +2                   | 781.82           | 79.55 |                  |
| NCM-H <sub>2</sub>   | 0                    | 778.72           | 25.02 | 12, 15, 16       |
|                      | +2                   | 781.65           | 74.98 |                  |
| NCM-CO               | 0                    | 778.75           | 22.05 | 12, 15, 16       |
|                      | +2                   | 781.3            | 77.95 |                  |

**Table S3** Assignment analysis of Mn in the XPS spectra of raw material and roasting products. (650 °C, 6h)

| Sample               | Mn 2p <sub>3/2</sub> |                  |        |               |
|----------------------|----------------------|------------------|--------|---------------|
|                      | Valence state        | Peak position/eV | At%    | References    |
| NCM-Raw              | +3                   | 641.12           | 44.66  | 3, 11, 14, 16 |
|                      | +4                   | 642.92           | 55.34  |               |
| NCM-Air              | +3                   | 641.13           | 69.37  | 2, 3, 7, 11   |
|                      | +4                   | 642.98           | 30.63  |               |
| NCM-H <sub>2</sub> O | +3                   | 641.27           | 100.00 | 3, 7          |
| NCM-N <sub>2</sub>   | +2                   | 640.76           | 100.00 | 7, 15         |
| NCM-CO <sub>2</sub>  | +2                   | 640.97           | 100.00 | 7, 15         |
| NCM-H <sub>2</sub>   | +2                   | 640.56           | 100.00 | 7, 15         |
| NCM-CO               | +2                   | 640.52           | 100.00 | 7, 15         |

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