# **Supporting Information**

# **Improved electrochemical performance of Li-Rich Cathode Materials via Spinel Li2MoO4 Coating**

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#### **Table S1.** Composition of cational elements in sample Pristine, 1wt%, 3wt% and 5wt% as measured by ICP-OES.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Samples | Sampling quality(g) | Constant volume(mL) | Measured element | Instrument reading(mg/L) | Converted content(mg/kg) | Sample element content(%) |
| Pristine | 0.0548 | 25 | Li | 2.011 | 91734.5 | 9.17% |
| 0.0548 | 25 | Li | 2.011 | 91723.9 | 9.17% |
| 0.0548 | 25 | Mn | 7.587 | 346126.4 | 34.61% |
| 0.0548 | 25 | Mn | 7.584 | 345969.7 | 34.60% |
| 0.0548 | 25 | Co | 1.978 | 90258.6 | 9.03% |
| 0.0548 | 25 | Co | 1.979 | 90285.8 | 9.03% |
| 0.0548 | 25 | Ni | 1.701 | 77585.9 | 7.76% |
| 0.0548 | 25 | Ni | 1.710 | 78006.2 | 7.80% |
| 1wt% | 0.0644 | 25 | Mo | 1.352 | 5248.0 | 0.52% |
| 0.0644 | 25 | Mo | 1.358 | 5271.7 | 0.53% |
| 3wt% | 0.0557 | 25 | Mo | 3.430 | 15394.1 | 1.54% |
| 0.0557 | 25 | Mo | 3.429 | 15389.2 | 1.54% |
| 5wt% | 0.0486 | 25 | Mo | 5.057 | 26011.3 | 2.60% |
| 0.0486 | 25 | Mo | 5.061 | 26032.0 | 2.60% |

#### **Table S2.** ICP-OES results of the obtained samples.

|  |  |  |
| --- | --- | --- |
|  | Target material | ICP data |
| Pristine | Li1.2Mn0.54Co0.13Ni0.13O2 | Li1.127Mn0.537Co0.131Ni0.113O2 |
| Mass proportion of Li2MoO4 coating layer |
| Designed | 1wt% | 3wt% | 5wt% |
| ICP data | 0.95wt% | 2.79wt% | 4.71wt% |

The design value is the mass fraction of (NH4)2MoO4 relative to Li-rich materials, while the experimental value is the mass fraction of Li2MoO4 relative to the overall sample.



#### **Figure S1.** XRD spectrum analysis of spinel Li2MoO4 phase.

The peaks observed near 18, 30, and 35° are completely matched with the peaks of pure Li2MoO4 with spinel Fd-3m crystal structure (sd\_0307446), and based on the good water solubility of Li2MoO4, the peak of Li2MoO4 disappears after washing with deionized water [1].

<https://materials.springer.com/isp/crystallographic/docs/sd_0307446>



#### **Figure S2.** SEM images for (a) Pristine, (b) 1wt%, (c) 3wt%, (d) 5wt%.



#### **Figure S3.** XPS spectra of (a) Mn 2p, (b) Co 2p, and (c) Ni 2p for Pristine and 3wt% sample.



#### **Figure S4.** The cyclic performance (a) and capacity retention rate (b) of four samples at 1C.

#### **References**

1. Zhu Z, Gao R, Waluyo I, Dong Y H, Hunt A, Lee J, Li J. Stabilized Co-Free Li-Rich Oxide Cathode Particles with An Artificial Surface Prereconstruction. Advanced Energy Materials, 2020, 10(35).