Electronic Supplementary Material (ESI) for RSC Advances.


# Supporting information

## The studying of the structure-activity relationship of electrochemical performance and Li/Ni mixing of lithium-rich materials by neutron diffraction

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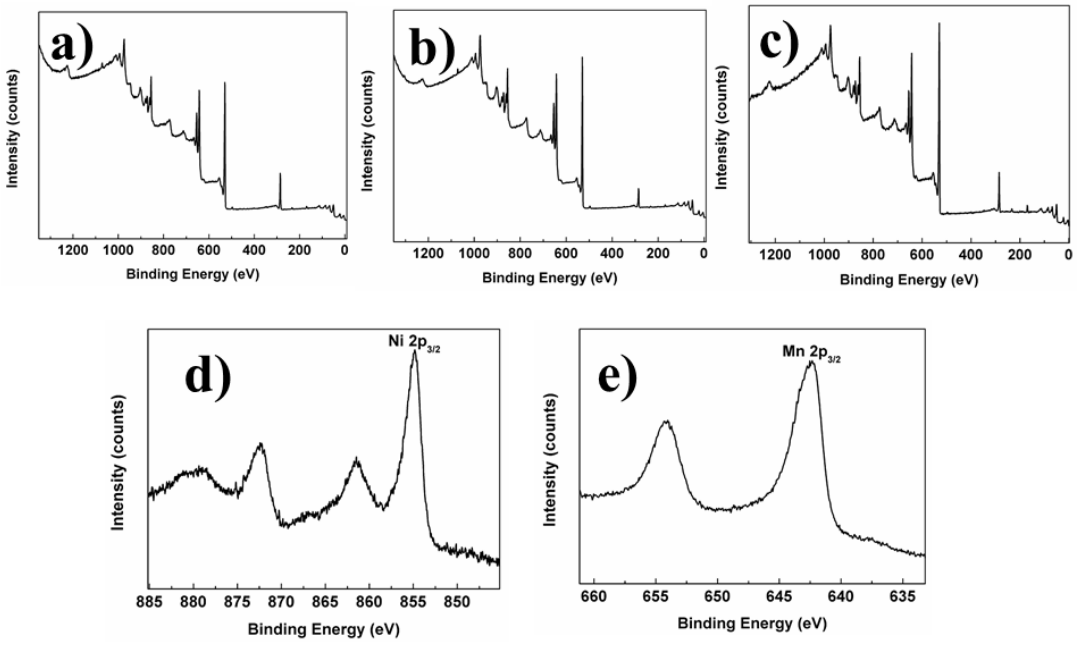


Figure SI 1. X-ray photoelectron spectroscopy (XPS) spectra of: a, d, e) pristine sample, b) 4mol% Mg-doped sample and c) 1mol% Al-doped sample.

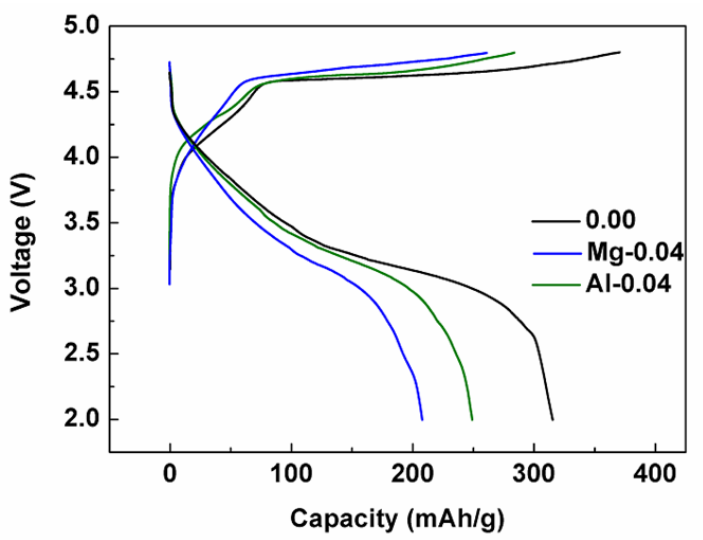


Figure SI 2. The first charge-discharge curves of the pristine, 4mol% Mg-doped and 1mol% Al-doped electrodes.

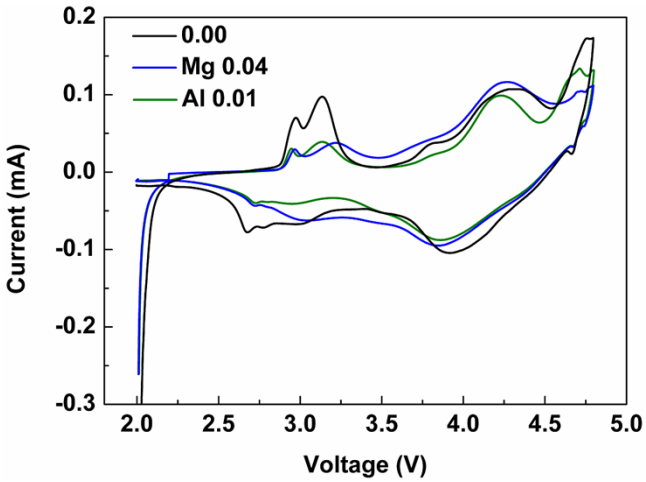


Figure SI 3. CV of the pristine, 4mol% Mg-doped and 1mol% Al-doped cathode materials in the voltage range between 2.0 and 4.8V, scan rate-0.1mV/s.

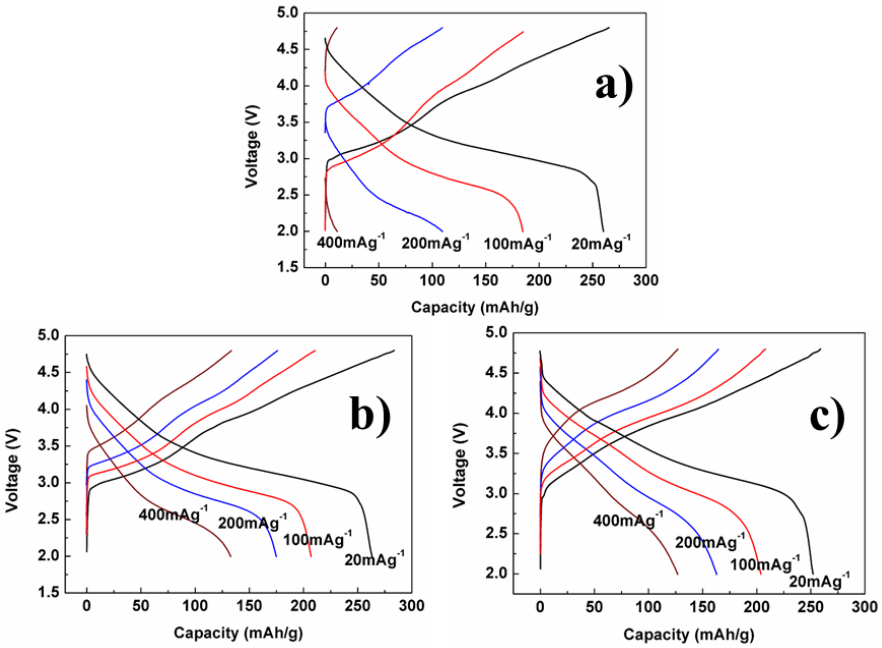


Figure SI 4. The charge-discharge curves of lithium-rich layered oxide materials at various rates between 2.0 and 4.8V: a) pristine electrode, b) 4mol% Mg-doped electrode and c) 1mol% Al-doped electrode.

Table SI 1. Discharge capacity of the pristine, 4mol% Mg-doped and 1mol% Al-doped samples at the current density of 100mAg$^{-1}$.

| Cycle | 3$^{rd}$ | 20$^{th}$ | 50$^{th}$ | 80$^{th}$ | Capacity retention (%) |
|---|---|---|---|---|---|
| Pristine (mAhg$^{-1}$) | 136 | 141 | 138 | 140 | 103 |
| 4mol% Mg-doped(mAhg$^{-1}$) | 184 | 183 | 193 | 188 | 102 |
| 1mol% Al-doped(mAhg$^{-1}$) | 180 | 179 | 174 | 170 | 94 |

Table SI 2. The discharge capacity of the pristine, 4mol% Mg-doped and 1mol% Al-doped samples at different charge-discharge current density.

| Rate | 20mAg$^{-1}$ | 100mAg$^{-1}$ | 200mAg$^{-1}$ | 400mAg$^{-1}$ |
|---|---|---|---|---|
| Pristine (mAhg$^{-1}$) | 261 | 140 | 110 | 10 |
| 4mol% Mg-doped(mAhg$^{-1}$) | 252 | 188 | 175 | 135 |
| 1mol% Al-doped(mAhg$^{-1}$) | 242 | 170 | 165 | 127 |