

Supporting Information

Unsaturated coordination modulation and enlarged pore size in nanoflower-like metal organic frameworks for enhanced lithium-oxygen battery performance

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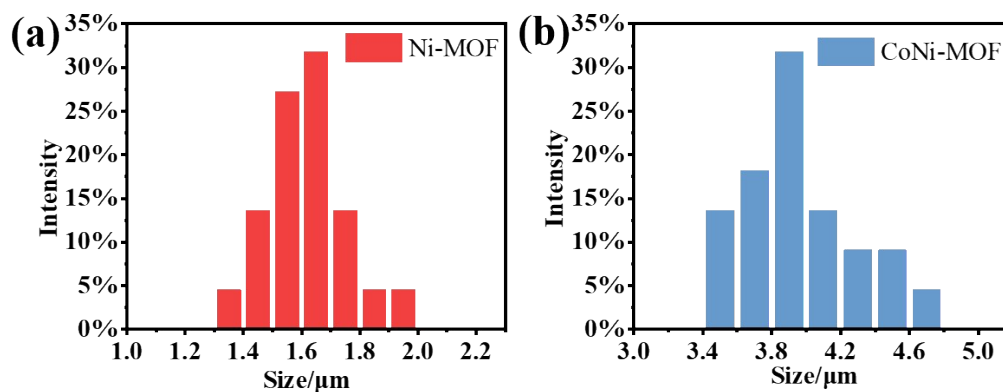


Fig. S1 Particle Size Distribution of (a) Ni-MOF and (b) CoNi-MOF.

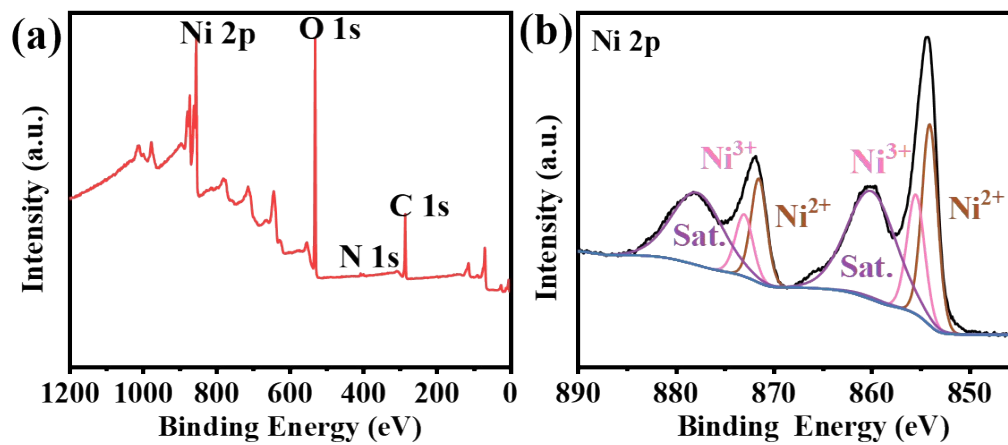


Fig. S2 (a)XPS survey and (b) high-resolution XPS spectra of Ni 2p of Ni-MOF.

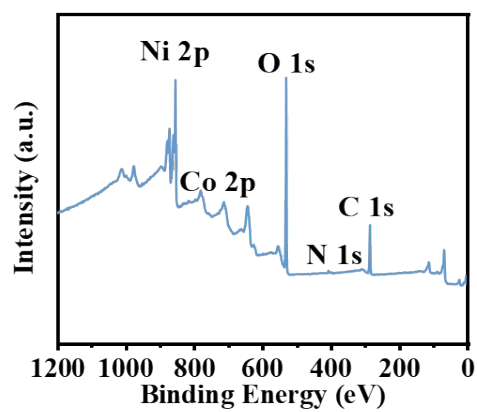


Fig. S3 XPS survey of CoNi-MOF.

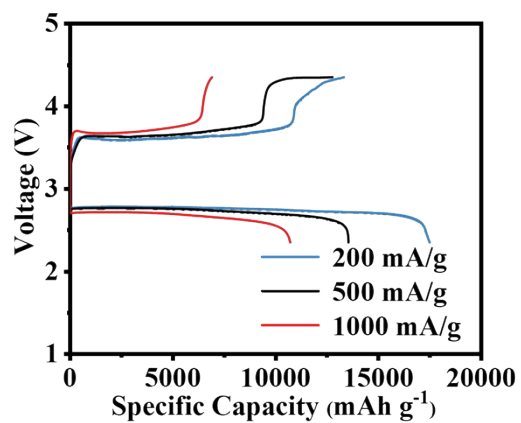


Fig. S4 Discharge/charge curves of Ni-MOF cathode at different current densities.

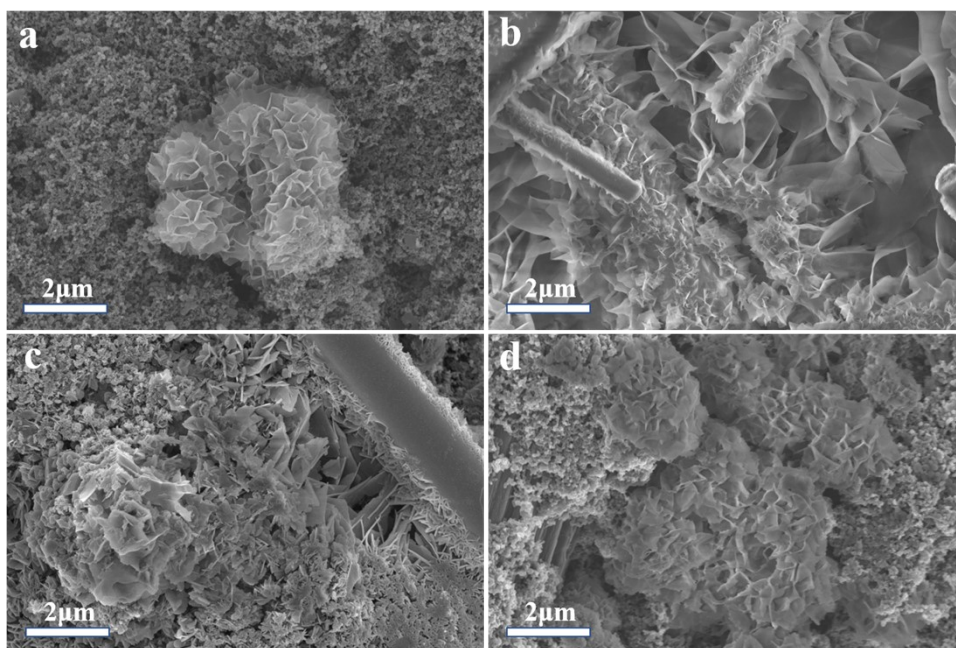


Fig. S5 SEM images of the Ni-MOF cathodes: (a) fresh cathode, (b) discharge to 600 mAh g⁻¹, (c) discharge to 2000 mAh g⁻¹ and (d) recharge to 2000 mAh g⁻¹.

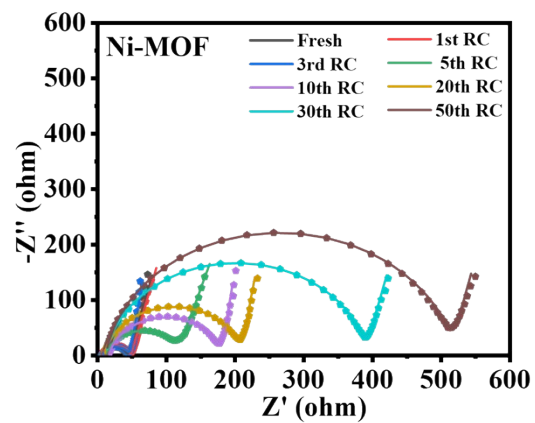


Fig. S6 EIS spectra of Ni-MOF electrodes at different states.

Table S1 ICP test results of CoNi-MOF.

| Sample | Element | Sample element content | Sample element content |
|----------|---------|------------------------|------------------------|
| | | C _x (mg/kg) | W (%) |
| CoNi-MOF | Co | 66808.9 | 6.68 |
| | Ni | 508563.7 | 50.86 |

Table S2 Oxidation states of Ni and Co ions in different states.

| | Ni ²⁺ /% | Ni ³⁺ /% | Co ²⁺ /% | Co ³⁺ /% |
|-----------|---------------------|---------------------|---------------------|---------------------|
| State I | 80.64 | 19.36 | 32.43 | 67.57 |
| State II | 45.45 | 54.55 | 31.03 | 68.97 |
| State III | 39.17 | 60.83 | 54.64 | 45.36 |
| State IV | 78.76 | 21.24 | 46.24 | 53.76 |

Table S3. Parameter values of the fitted equivalent circuit for Ni-MOF electrodes.

| States | R_s (Ω) | R_{ct} (Ω) | CPE ($\Omega^{-1} \text{ cm}^{-2} \text{ s}^n$) | Z_W ($\Omega^{-1} \text{ cm}^{-2} \text{ s}^{0.5}$) |
|----------------------------|--------------------|-----------------------|--|--|
| Pristine | 7.737 | 35.31 | 0.91918 | 0.39973 |
| 1 st charged | 7.179 | 39.30 | 0.92793 | 0.291 |
| 3 rd Recharged | 7.989 | 35.94 | 0.88581 | 0.53135 |
| 5 th Recharged | 11.98 | 108.1 | 0.86533 | 0.80959 |
| 10 th Recharged | 16.64 | 164.8 | 0.8798 | 1.482 |
| 20 th Recharged | 10.54 | 200.4 | 0.91047 | 1.399 |
| 30 th Recharged | 12.4 | 378.7 | 0.91831 | 0.87578 |
| 50 th Recharged | 12.32 | 536.4 | 0.91525 | 2.715 |

Table S4. Parameter values of the fitted equivalent circuit for CoNi-MOF electrodes.

| States | R_s (Ω) | R_{ct} (Ω) | CPE ($\Omega^{-1} \text{ cm}^{-2} \text{ s}^n$) | Z_W ($\Omega^{-1} \text{ cm}^{-2} \text{ s}^{0.5}$) |
|----------------------------|--------------------|-----------------------|--|--|
| Pristine | 8.284 | 30.21 | 0.92134 | 0.61555 |
| 1 st charged | 7.779 | 30.86 | 0.91892 | 0.27749 |
| 3 rd Recharged | 9.463 | 35.32 | 0.89096 | 0.46002 |
| 5 th Recharged | 8.454 | 76.74 | 0.85982 | 0.6523 |
| 10 th Recharged | 12.06 | 103.7 | 0.86964 | 0.81394 |
| 20 th Recharged | 11.1 | 131.5 | 0.89444 | 0.88721 |
| 30 th Recharged | 10.26 | 195.2 | 0.90619 | 1.26 |
| 50 th Recharged | 13.81 | 230.2 | 0.9152 | 1.721 |