

## Supplementary Information

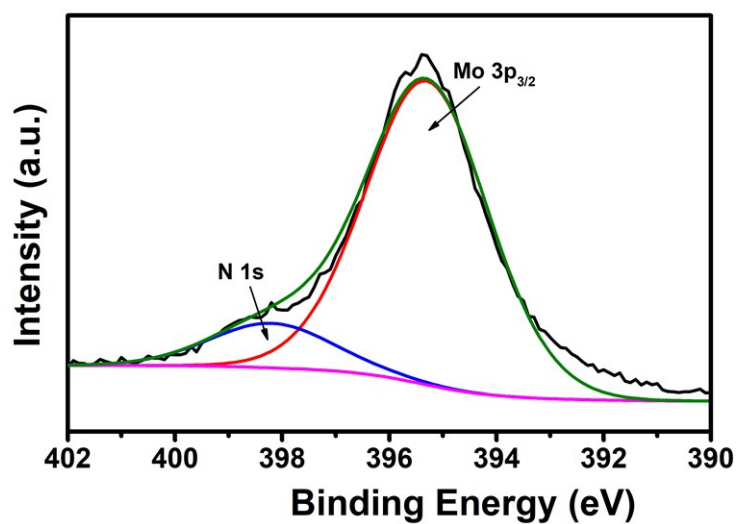
### Hexagonal MoO<sub>3</sub> as Zinc Intercalation Anode towards Zinc Metal-Free Zinc-Ion Battery

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Xue<sup>\* a</sup>

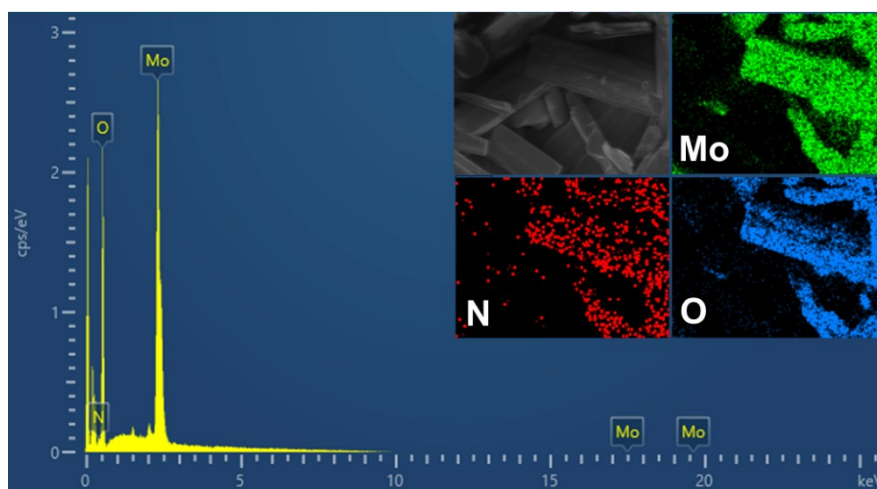
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**Fig. S1** N 1s and Mo 3p<sub>3/2</sub> XPS of the as-prepared h-MoO<sub>3</sub>.



**Fig. S2** EDX-mapping result for the as-prepared h-MoO<sub>3</sub>.

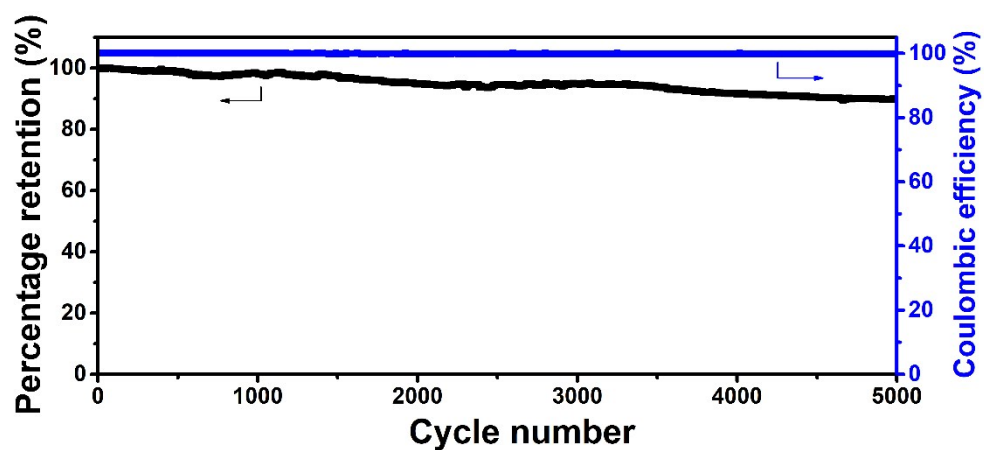


Fig. S3 The cyclic stability and Coulombic efficiency of Zn//h-MoO<sub>3</sub> cell at 2 A g<sup>-1</sup>.

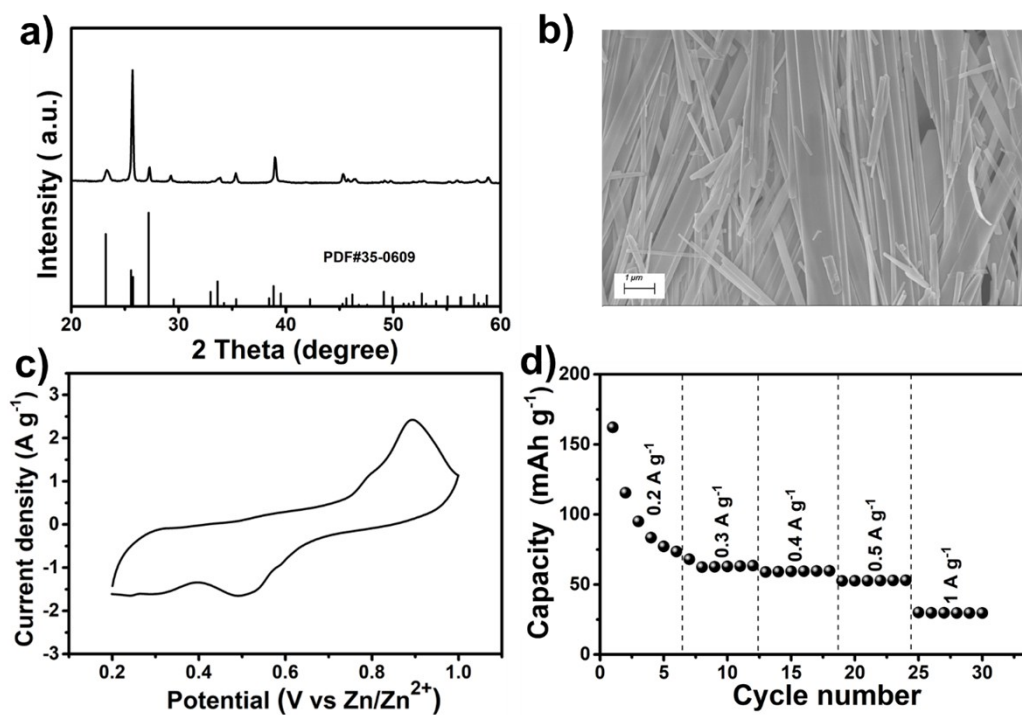
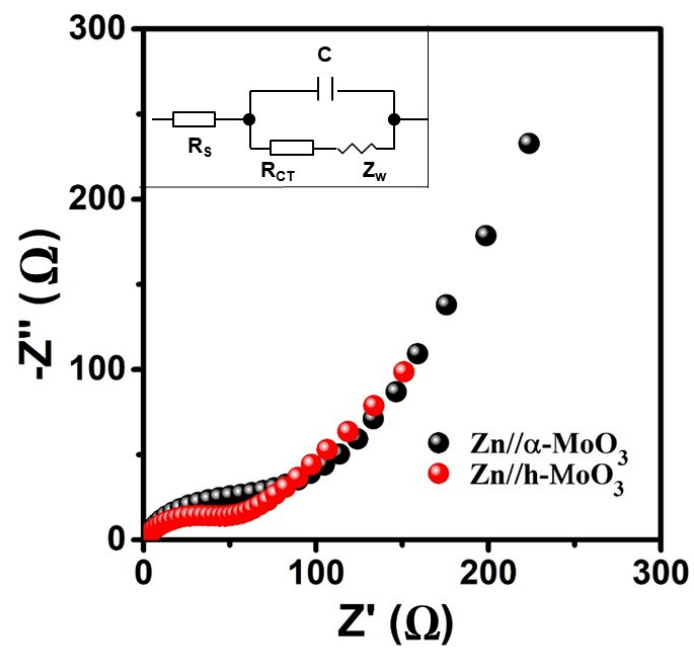
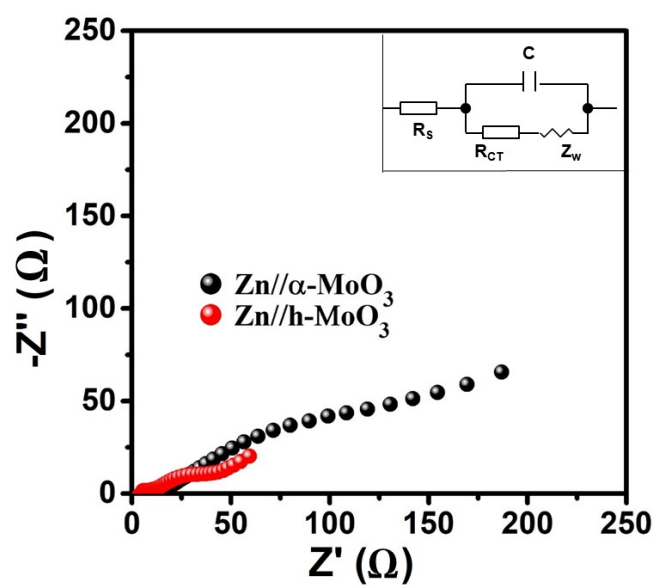


Fig. S4 a) XRD, b) SEM of the as-prepared  $\alpha$ -MoO<sub>3</sub>, c) CV, d) Rate performance of the Zn// $\alpha$ -MoO<sub>3</sub> cell.



**Fig. S5** Nyquist plots of the fresh Zn// $\alpha$ -MoO<sub>3</sub> and fresh Zn//h-MoO<sub>3</sub> cells.



**Fig. S6** Nyquist plots of the cycled Zn// $\alpha$ -MoO<sub>3</sub> and cycled Zn//h-MoO<sub>3</sub> cells.

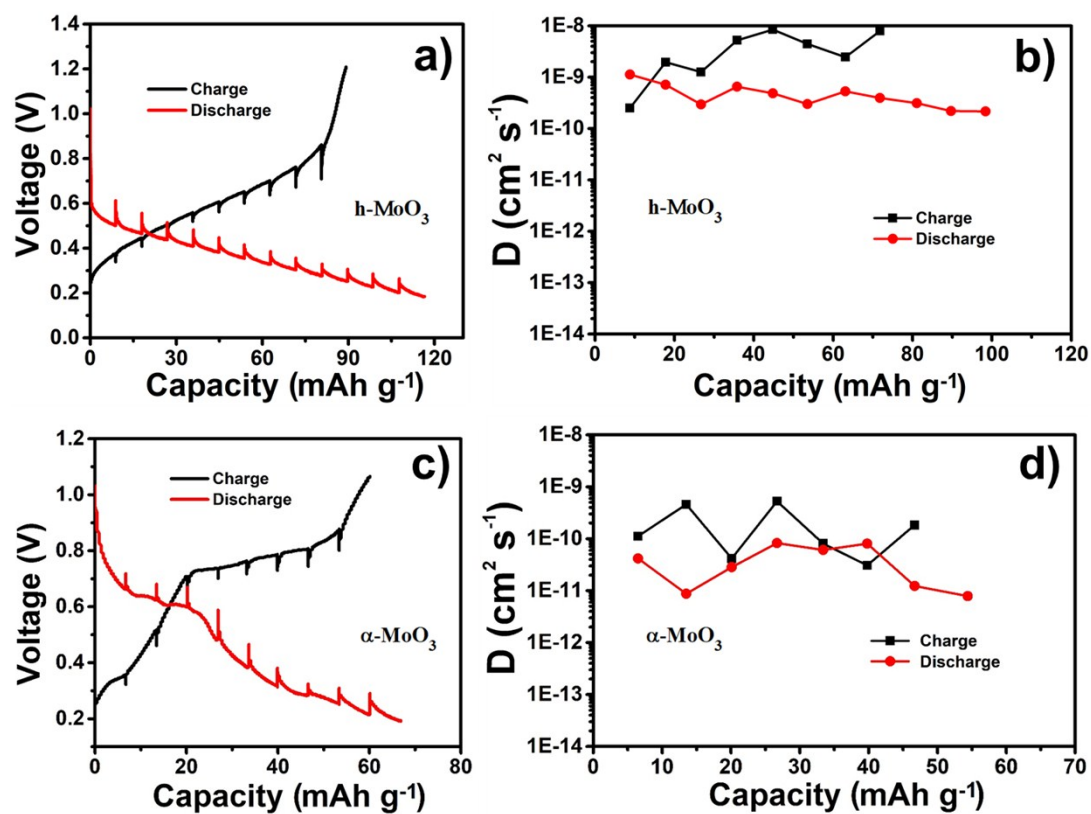


Fig. S7 GITT curves and diffusion coefficients of a),b) h-MoO<sub>3</sub> and c),d) α-MoO<sub>3</sub>.

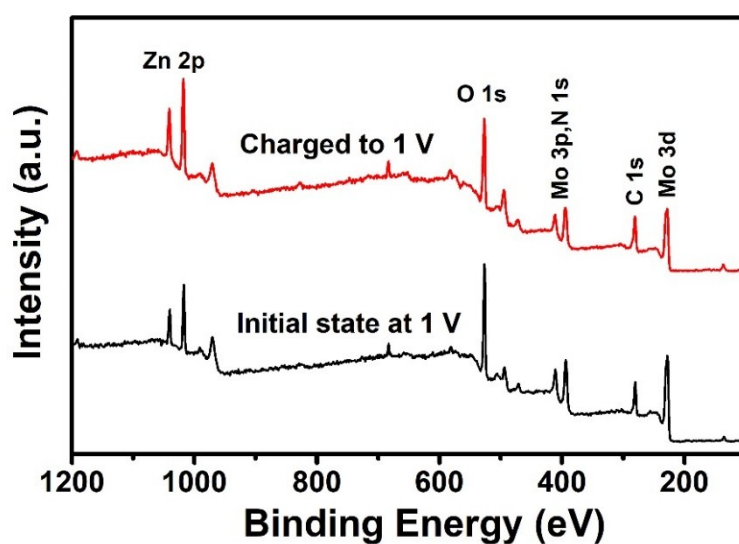


Fig. S8 XPS survey spectra of the h-MoO<sub>3</sub> at the initial state at 1V and the fully charged state at 1V.

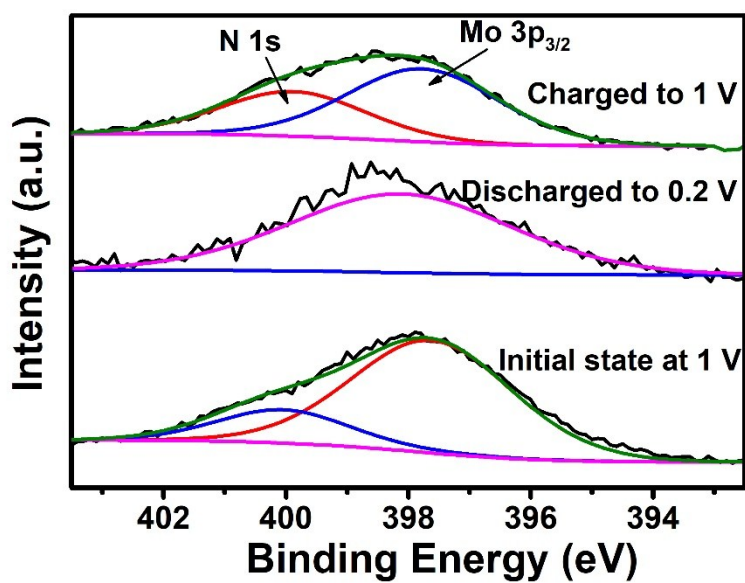


Fig. S9 N 1s XPS of the as-prepared h-MoO<sub>3</sub> at different states.

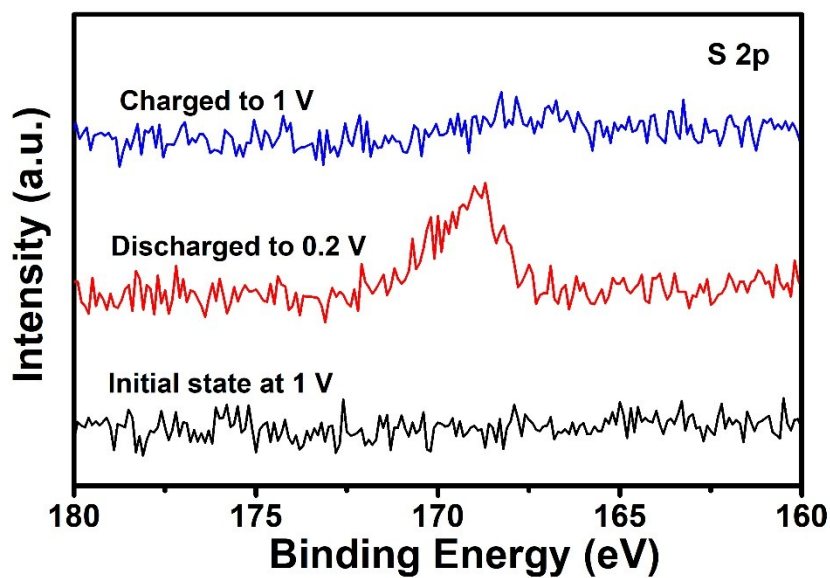
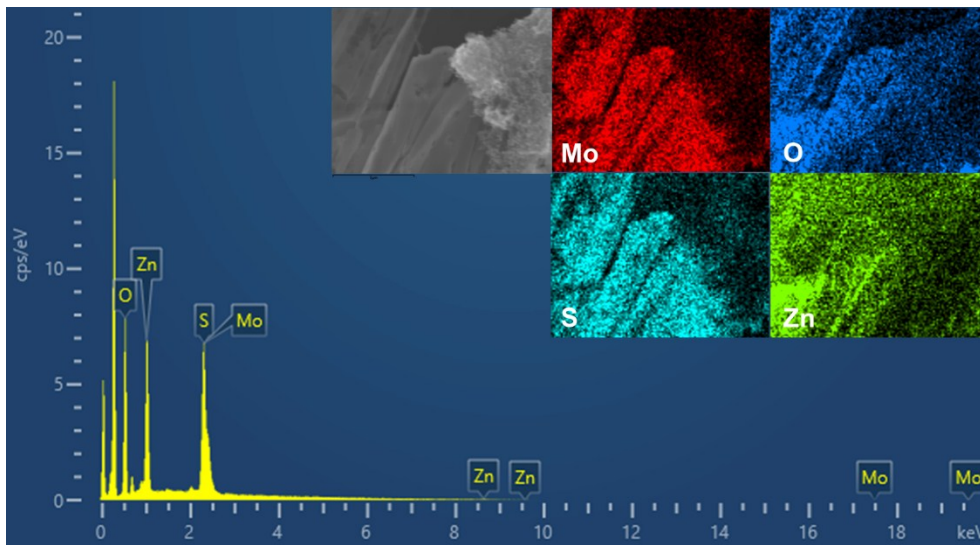
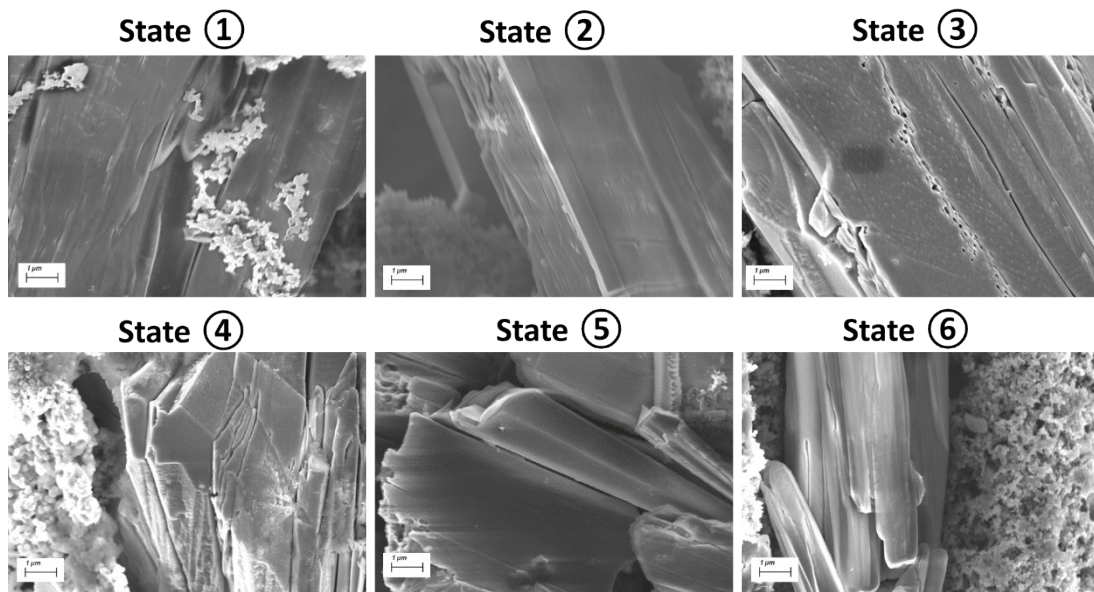


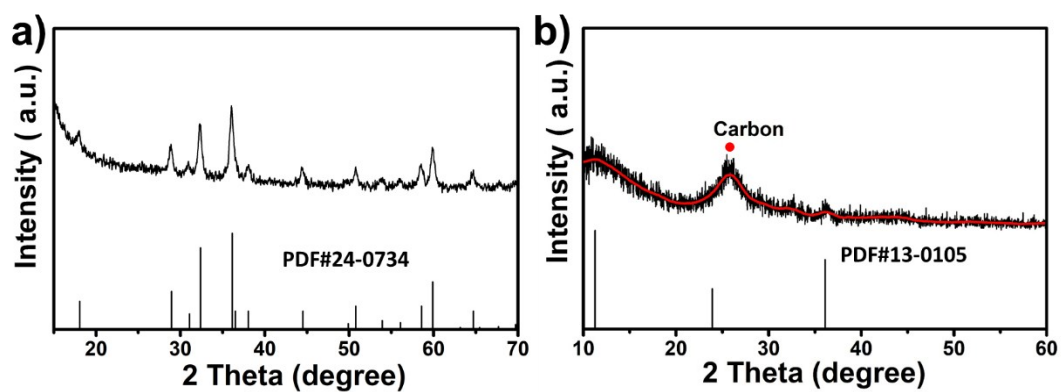
Fig. S10 S 2p XPS of the as-prepared h-MoO<sub>3</sub> at different states.



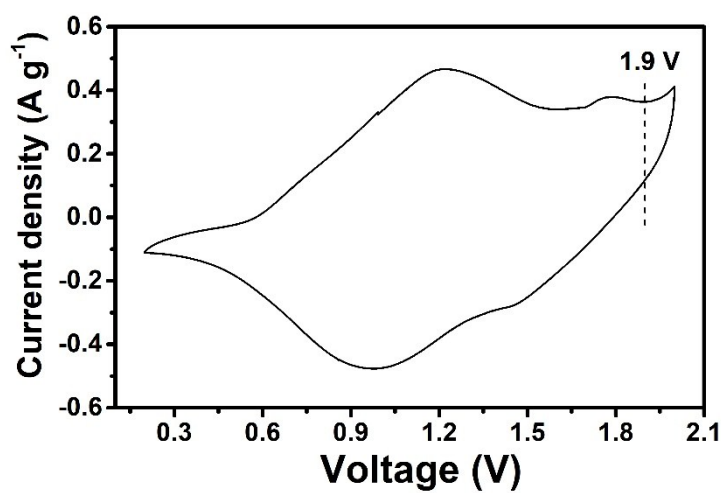
**Fig. S11** EDX mapping of the h-MoO<sub>3</sub> at the fully discharged state.



**Fig. S12** SEM images of the h-MoO<sub>3</sub> at various state in Fig. 2a.

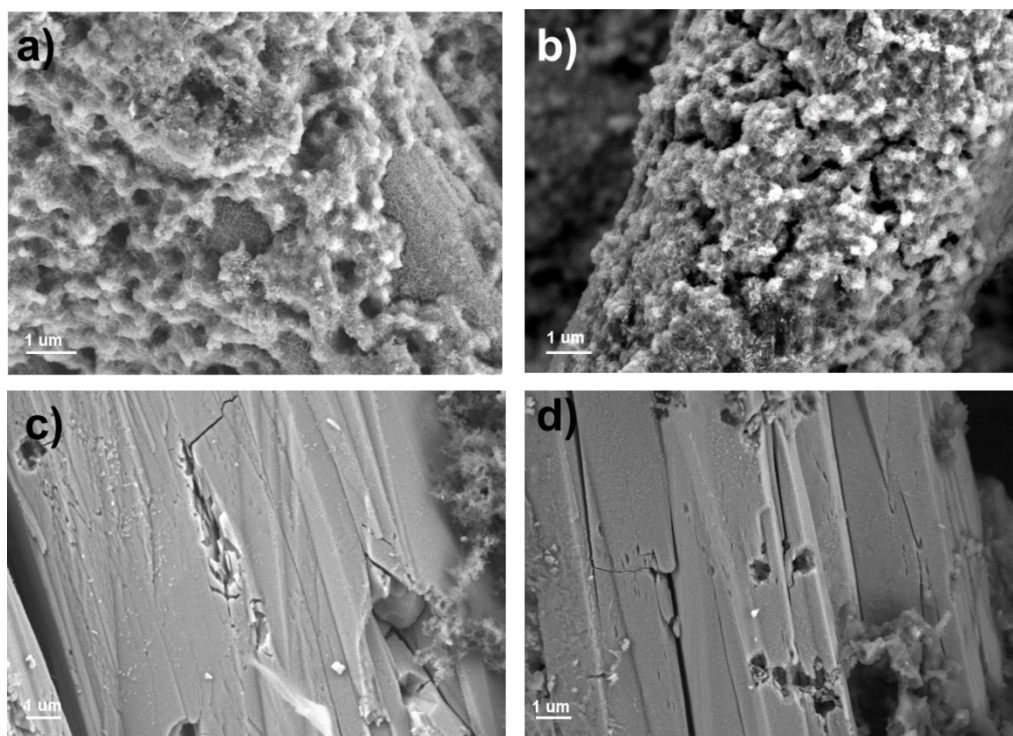


**Fig. S13** XRD of a)  $\text{Mn}_3\text{O}_4$  and b)  $\text{Zn}^{2+}$ -intercalated  $\text{MnO}_2$  (denoted as  $\text{Zn}_{0.2}\text{MnO}_2$ ).



**Fig. S14** CV curve of  $\text{h-MoO}_3//\text{Zn}_{0.2}\text{MnO}_2$  battery at  $1 \text{ mV s}^{-1}$  in the voltage of 0.2-2.0 V.





**Fig. S15** SEM images of the a) discharged  $Zn_{0.2}MnO_2$ , b) charged  $Zn_{0.2}MnO_2$ , c) discharged h- $MoO_3$ , and d) charged h- $MoO_3$ .

**Table S1.** Comparison of the batteries performance parameters for Zn metal batteries and our zinc metal free battery.

Active material (active mass)	Electrolytes	Potential window	Capacity (based on the mass of cathode)	Capacity (based on the mass of cathode and anode)	Ref.
Zn//polyaniline-intercalated MnO <sub>2</sub>	2M ZnSO <sub>4</sub> + 0.1M MnSO <sub>4</sub>	1–1.8 V	280 mA h g <sup>-1</sup> at 0.2 A g <sup>-1</sup>	1.1 mA h g <sup>-1</sup> at 0.2 A g <sup>-1</sup>	1
Zn//NaV <sub>3</sub> O <sub>8</sub> ·1.5H <sub>2</sub> O	1M ZnSO <sub>4</sub> + 1M Na <sub>2</sub> SO <sub>4</sub>	0.3–1.25 V	380 mA h g <sup>-1</sup> at 0.1 A g <sup>-1</sup>	1.5 mA h g <sup>-1</sup> at 0.1 A g <sup>-1</sup>	2
Zn//Co <sub>0.247</sub> V <sub>2</sub> O <sub>5</sub> ·0.944H <sub>2</sub> O	20M LiTFSI + 1M Zn (TFSI) <sub>2</sub>	0.6–2.2 V	15 Wh kg 432 mA h g <sup>-1</sup> at 0.1 A g <sup>-1</sup>	1.7 mA h g <sup>-1</sup> at 0.1 A g <sup>-1</sup>	3
Zn//vanadium oxynitride	3 M Zn (CF <sub>3</sub> SO <sub>3</sub> ) <sub>2</sub>	0.2–1.8 V	15 Wh kg 603 mAh g <sup>-1</sup> at 0.2C	2.4 mAh g <sup>-1</sup> at 0.2C	4
Zn//oxygen-deficient V <sub>6</sub> O <sub>13</sub>	3 M Zn(TFSI) <sub>2</sub>	0.2–1.5 V	15 Wh kg 401 mA h g <sup>-1</sup> at 0.2 A g <sup>-1</sup>	1.6 mA h g <sup>-1</sup> at 0.2 A g <sup>-1</sup>	5
Zn//E-MoS <sub>2</sub>	1 M ZnSO <sub>4</sub>	0–1.3 V	15 Wh kg 202.6 mA h g <sup>-1</sup> at 0.1 A g <sup>-1</sup>	0.8 mA h g <sup>-1</sup> at 0.1 A g <sup>-1</sup>	6
Zn//V <sub>2</sub> O <sub>5</sub> nanopaper	2 M ZnSO <sub>4</sub>	0.2–1.6V	375 mAh g <sup>-1</sup> at 0.5 A g <sup>-1</sup>	1.5 mAh g <sup>-1</sup> at 0.5 A g <sup>-1</sup>	7
Zn//oxygen-deficient MnO <sub>2</sub>	1 M ZnSO <sub>4</sub> + 0.2M MnSO <sub>4</sub>	1–1.8 V	345 mAh g <sup>-1</sup> at 0.2 A g <sup>-1</sup>	1.4 mAh g <sup>-1</sup> at 0.2 A g <sup>-1</sup>	8
h-MoO <sub>3</sub> //Zn <sub>0.2</sub> MnO <sub>2</sub>	1 M ZnSO <sub>4</sub>	0.2–1.9 V	-	56.7 mAh g <sup>-1</sup> at 0.1 A g <sup>-1</sup>	This work

## References

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