

Supporting Information

Boosting the Capacity and Stability of MoO₃ Cathode via Valence Regulation and Polypyrrole Coating for Rechargeable Zn Ion Battery

Yachen He,^a Weiwei Xue,^a Yifeng Huang,^a Hongwei Tang,^a Guangxia Wang,^a Dezhou Zheng,^{*a} Wei Xu,^a Fuxin Wang^{*a}, Xihong Lu^{ab}

^aSchool of Applied Physics and Materials, Wuyi University, Jiangmen 529020, PR China. E-mail: wangfux91@126.com

^bMOE of the Key Laboratory of Bioinorganic and Synthetic Chemistry, The Key Lab of Low-carbon Chem & Energy Conservation of Guangdong Province, School of Chemistry, Sun Yat-Sen University, Guangzhou 510275, PR China

The specific capacity (C_m , mAh g⁻¹) is calculated by equation (1-1), where Δt (h) is the discharge time, I (mA) is the current density and m (g) is the loading mass of the active substance. All current densities in the article are related to the mass of the active material.

$$C_m = \frac{I \times \Delta t}{m} \quad (1-1)$$

Also, the energy density E_m (Wh kg⁻¹) and power density (P , W kg⁻¹) can be calculated for different GCDs profiles according to the following equation, where U (V) is the voltage window

$$E_m = \frac{I \int U dt}{m} \quad (1-2)$$

$$P = \frac{E_m}{t} \quad (1-3)$$

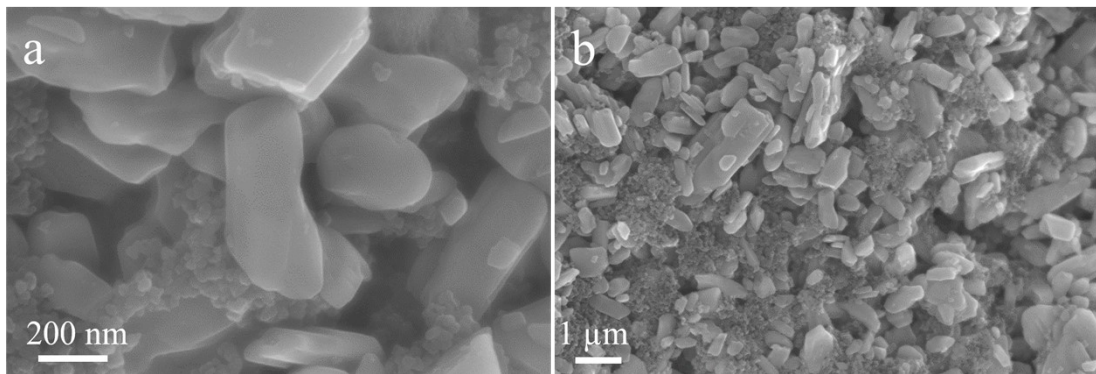


Figure S1 SEM images of commercial MoO₃.

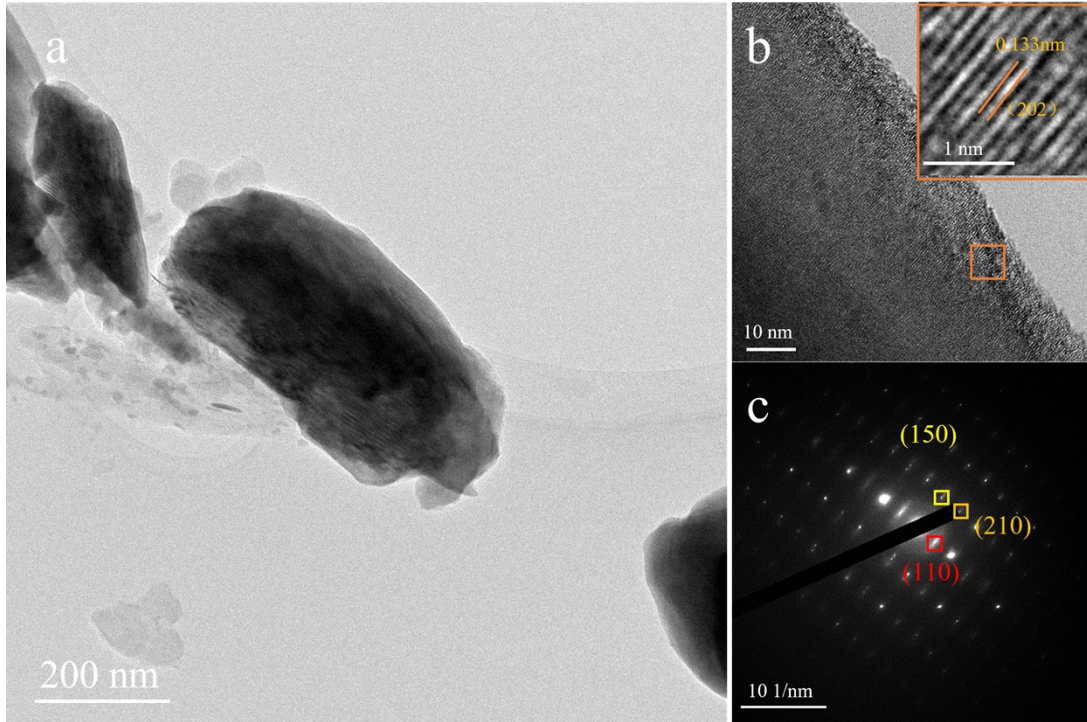


Figure S2 (a) TEM, (b) HRTEM, and (c) SAED images of commercial MoO_3 .

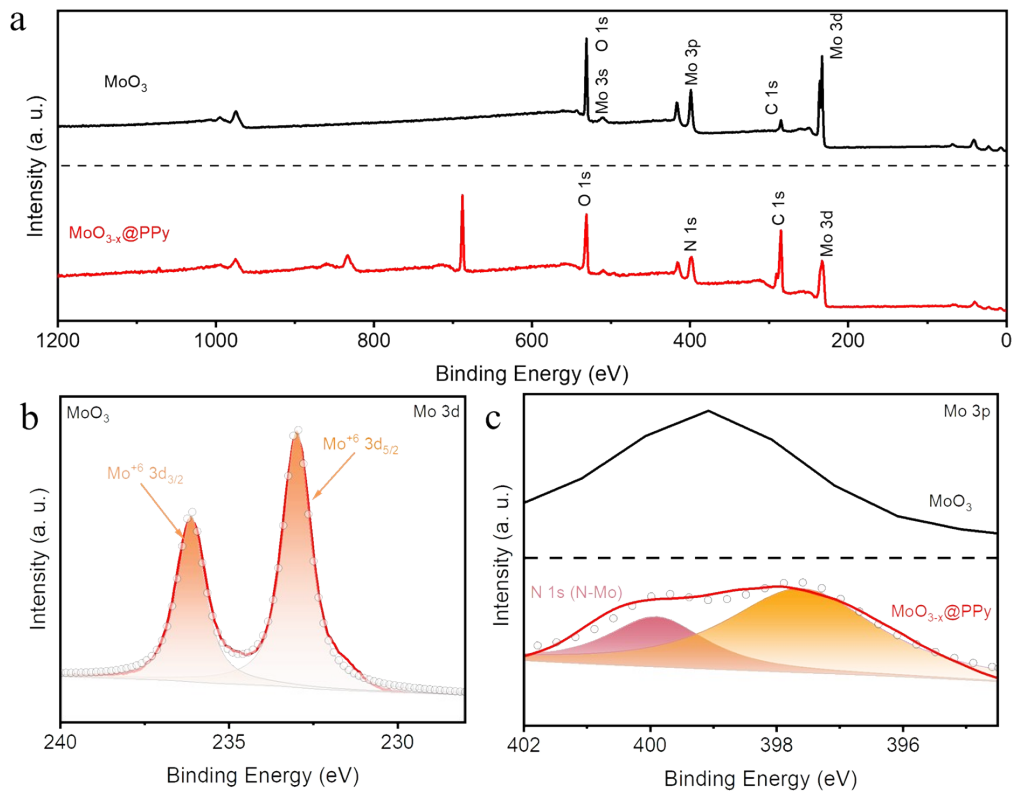


Figure S3 (a) The XPS survey spectra of the $\text{MoO}_{3-x}\text{@PPy}$ electrode materials. (b) Mo 3d spectra of the MoO_3 sample. (c) XPS spectra of the Mo $3p_{3/2}$ and N 1s orbitals of MoO_3 and $\text{MoO}_{3-x}\text{@PPy}$

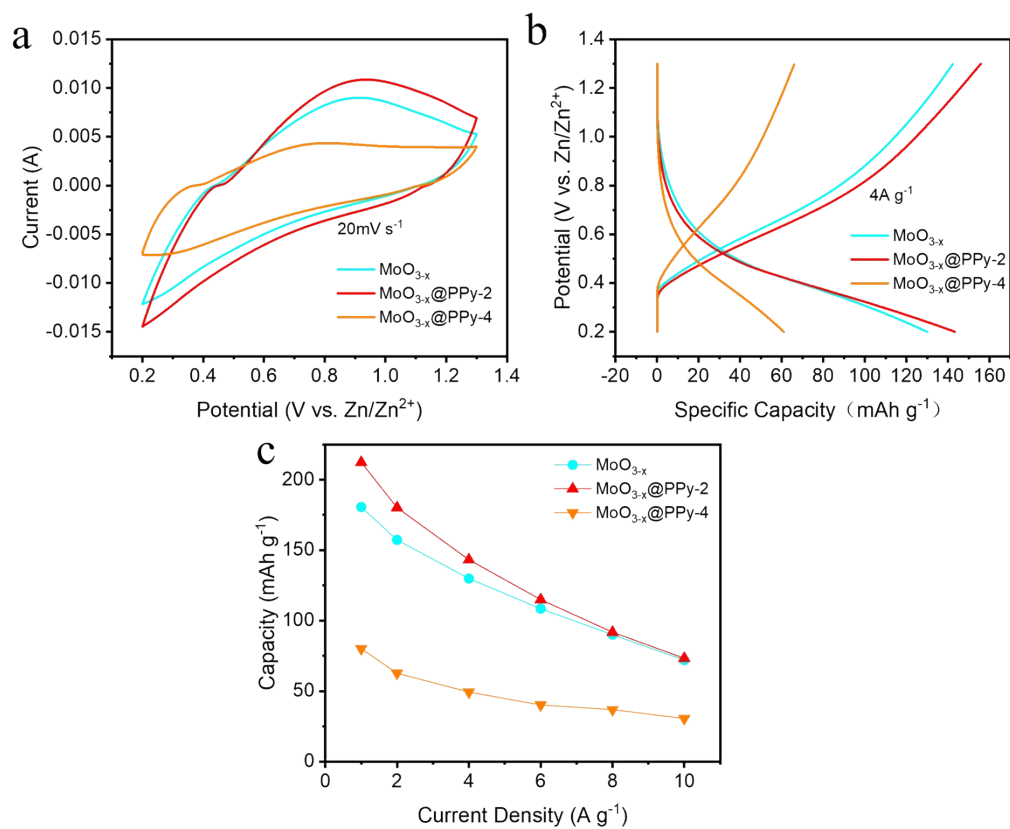


Figure S4 (a, b) CV and GCD curves for all batteries at a scan rate of 20 mV s⁻¹ and a current density of 4 A g⁻¹. (b) Rate performance of Zn//MoO_{3-x} and Zn//MoO_{3-x}@PPy batteries with different thicknesses of PPy layers electrodeposited.

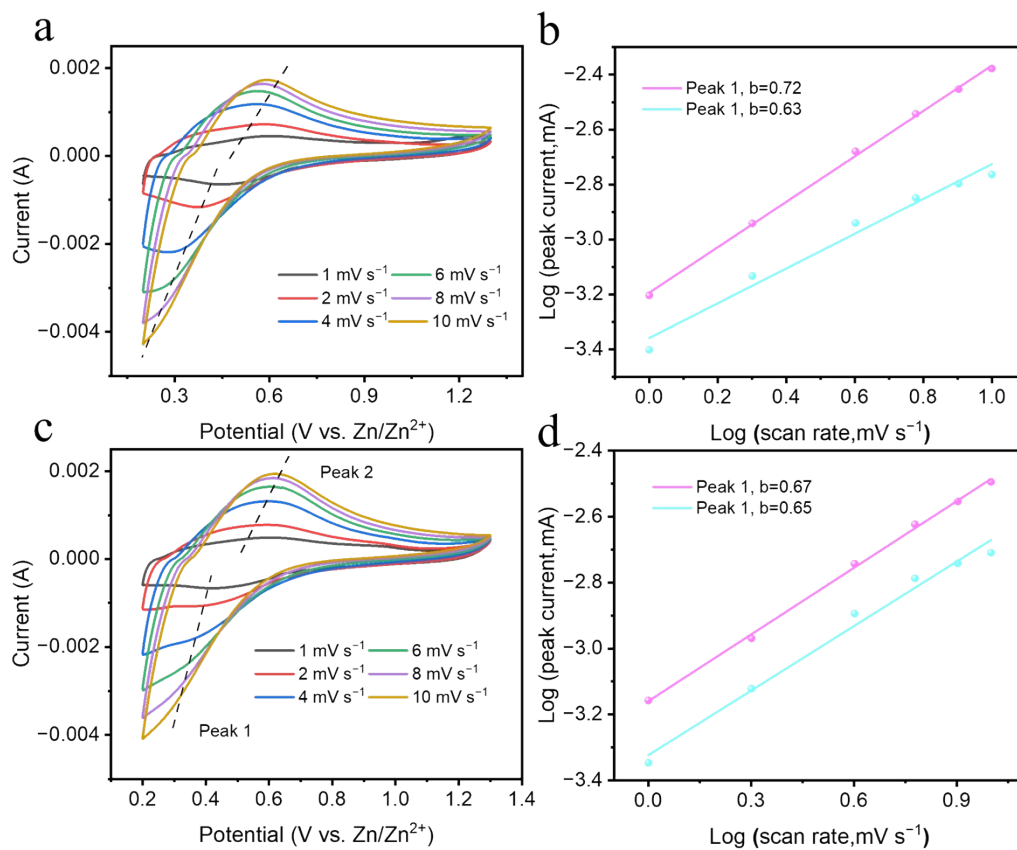


Figure S5 (a, c) CV curves for MoO_3 and MoO_{3-x} at a range of scan rates of 1, 2, 4, 6, 8 and 10 mV s^{-1} . (b, d) $\log(i)$ vs $\log(v)$ plots of the two peaks in the CV curve for MoO_3 and MoO_{3-x} .

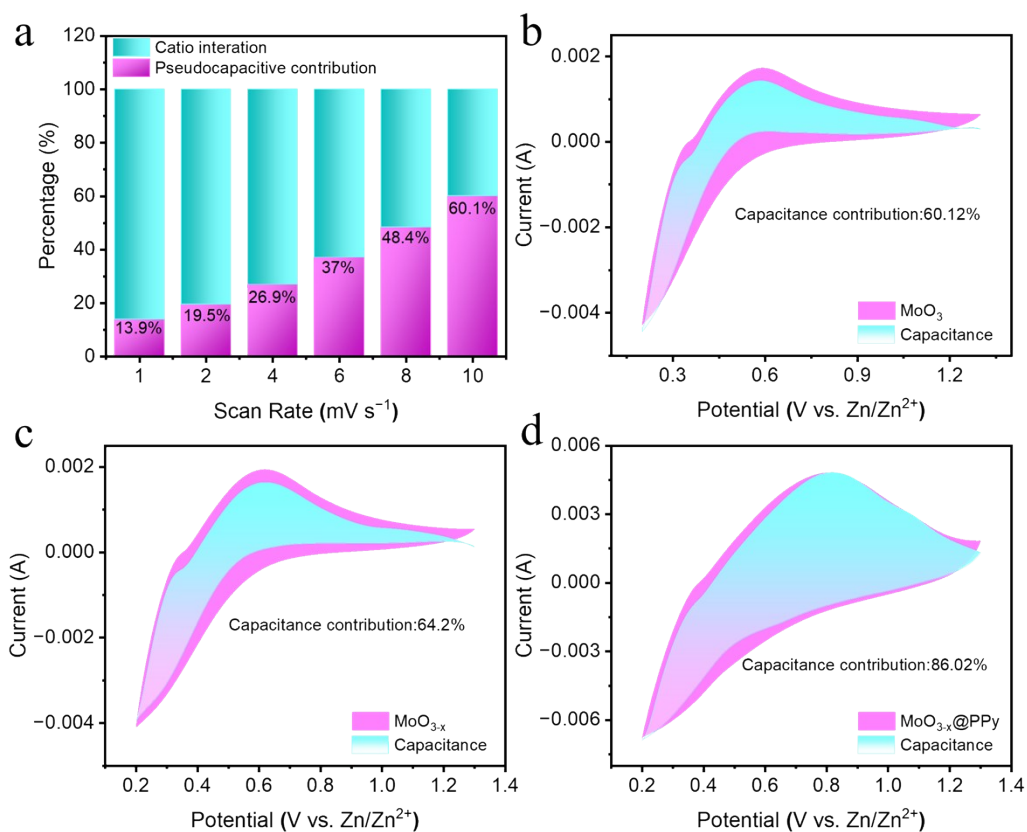


Figure S6 (a) Ratio of diffusion contribution and capacitance contribution of Zn//MoO₃ and (b, c, and d) Capacitive contribution (inset) and diffusion contribution of MoO₃, MoO_{3-x} and MoO_{3-x}@PPy electrodes at 10 mV s⁻¹.

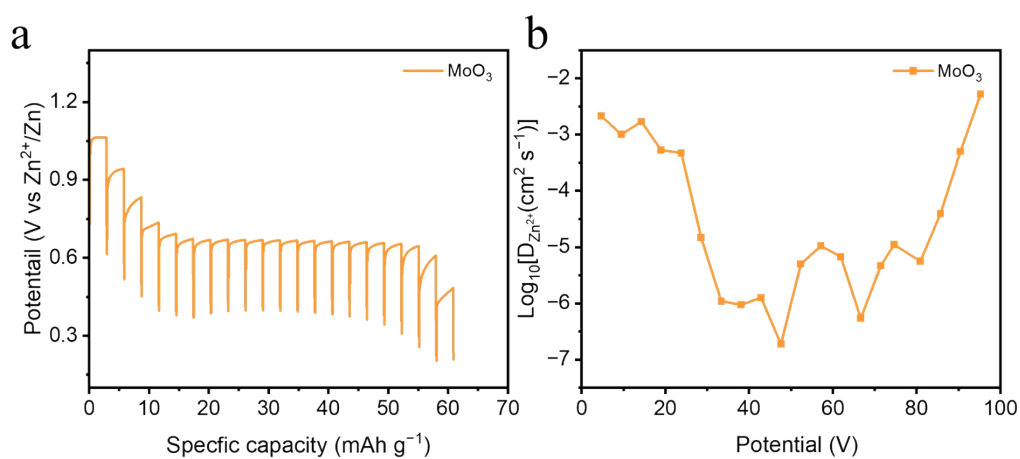


Figure S7 (a) Discharge GITT curves for Zn//MoO₃ at a current density of 2 A g⁻¹ and (b) corresponding Zn²⁺ coefficients $D_{Zn^{2+}}$.