

Supporting Information for

A “one-for-three” Strategy through a Facile One-step Hydrothermal Engineering of Commercial MoO₃ for High-Performance Proton Storage

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Calculation of specific gravimetric capacitance, energy density and power density

The specific of gravimetric capacitance are determined by the following calculation

formulas:

$$C_s = \frac{I \times \Delta t}{m \times \Delta V} \quad (1)$$

Where C_s ($F g^{-1}$) is the specific gravimetric capacitance, I (A) is the discharge current, Δt (s) is the discharge time, m (g) is the full mass of the active materials.

The energy density and power density of the electrode in the symmetric supercapacitor is calculated by the following equation:

$$E = \frac{1}{2 \times 3.6} C_s \Delta V^2 \quad (2)$$

$$P = \frac{3600 \times E}{\Delta t} \quad (3)$$

E ($Wh kg^{-1}$) and P ($W kg^{-1}$) are the energy density and power density, respectively.

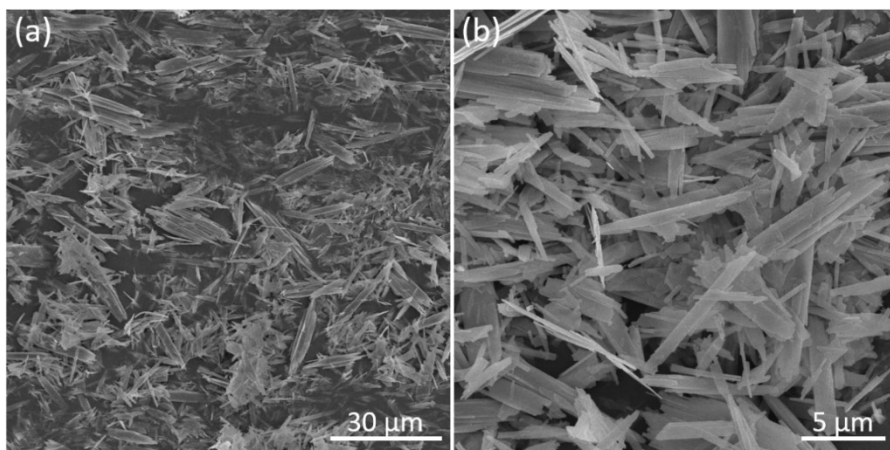


Fig. S1 (a, b) SEM images of P0-MoO₃ at different magnifications.

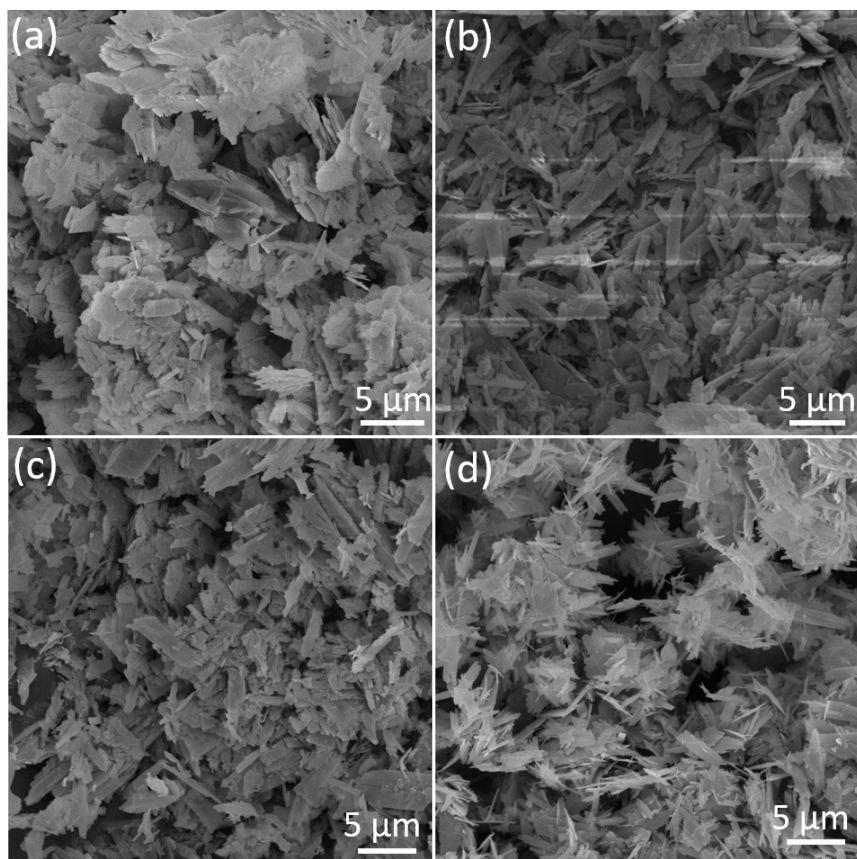


Fig. S2 SEM images of (a) P50-MoO₃, (b) P150-MoO₃, (c) P300-MoO₃, and (d) P500-MoO₃.

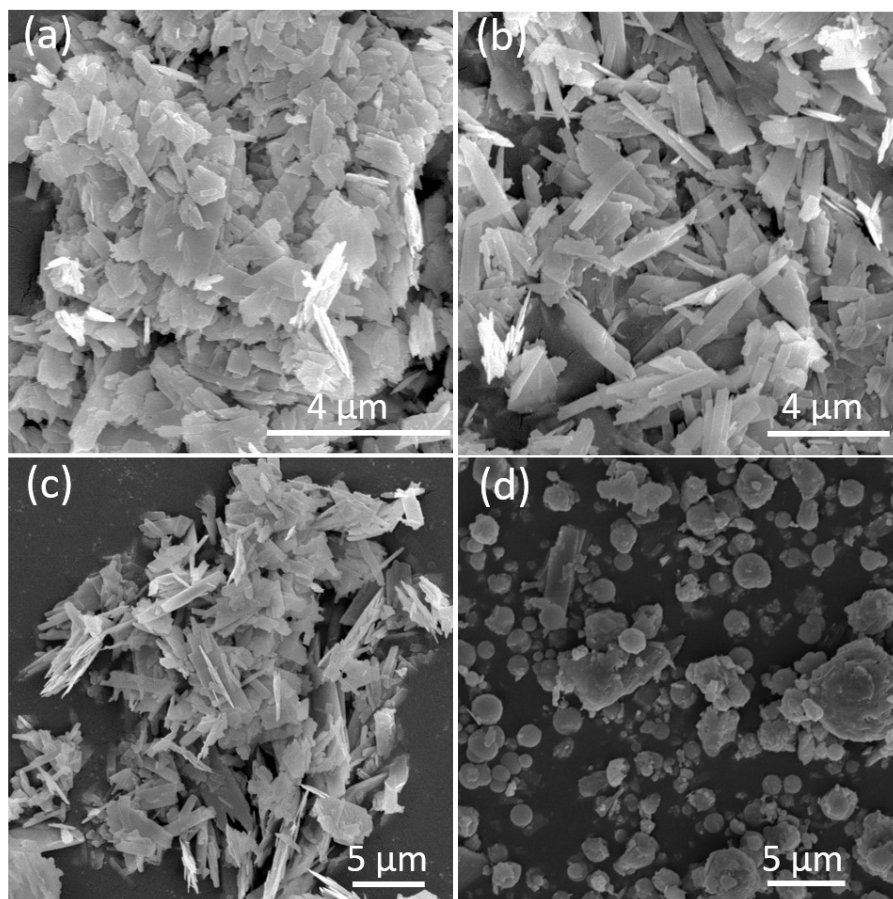


Fig. S3 SEM images of (a) PANI-MoO₃-80, (b) P100-MoO₃, (c) PANI-MoO₃-160, and (d) PANI-MoO₃-200.

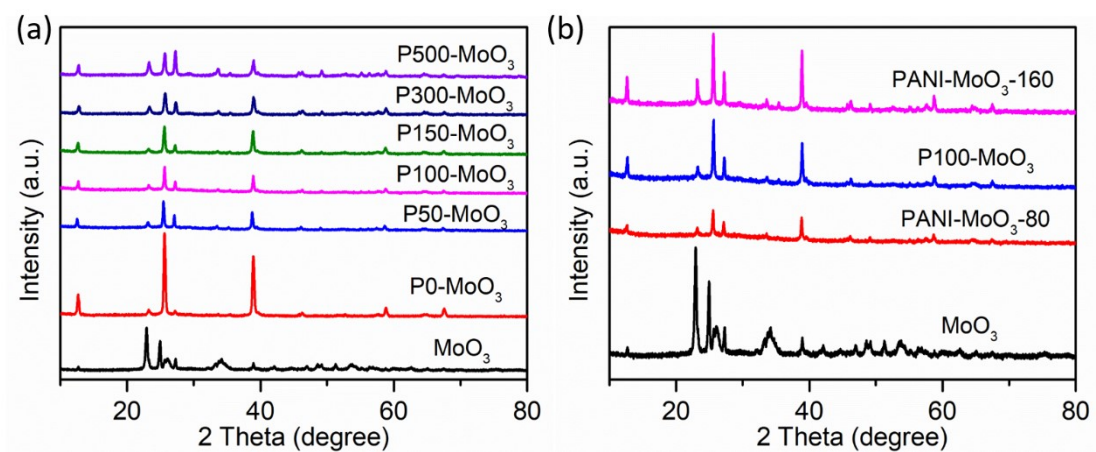


Fig. S4 XRD curves of MoO₃ with different (a) aniline monomers, and (b) hydrothermal temperatures.

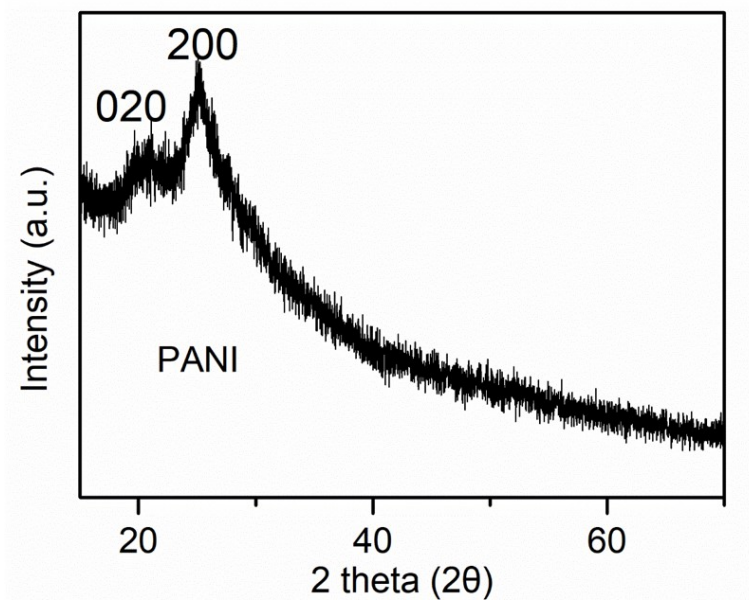


Fig. S5 XRD pattern of PANI.

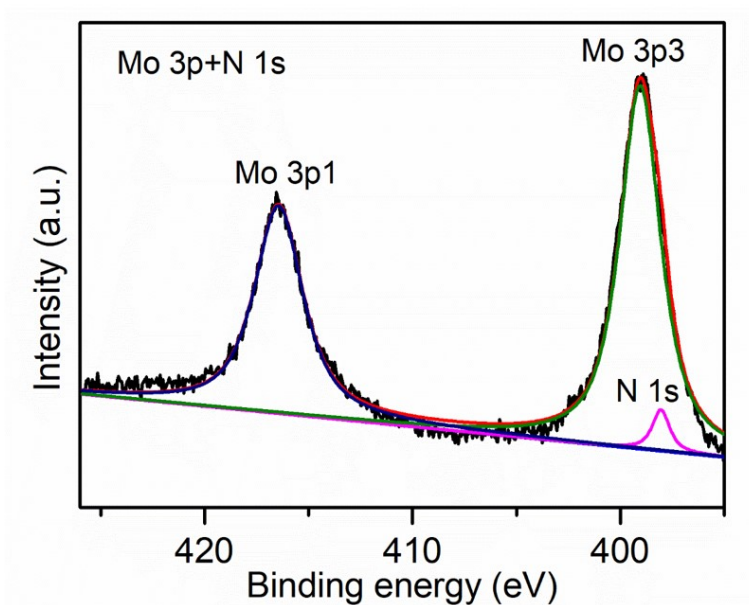


Fig. S6 XPS of P100-MoO₃ showing the Mo 3p and N1s.

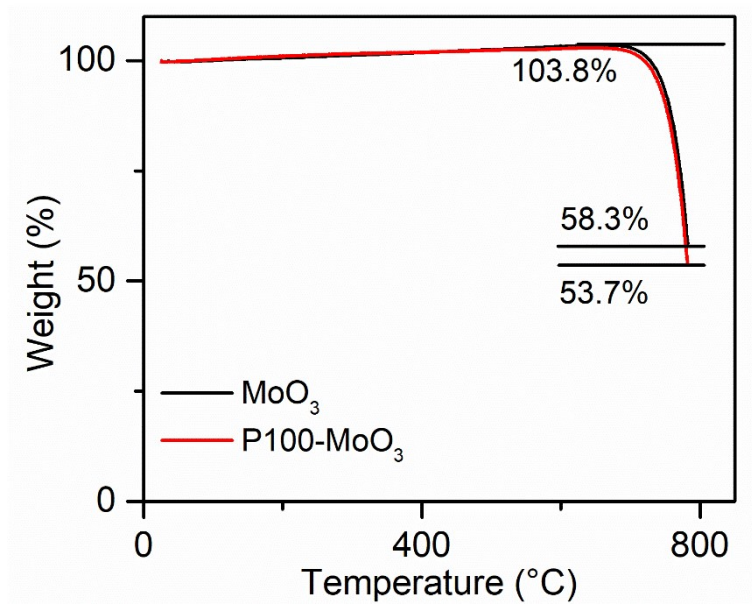


Fig. S7 Thermogravimetric analysis (TGA) of pristine MoO₃ and P100-MoO₃.

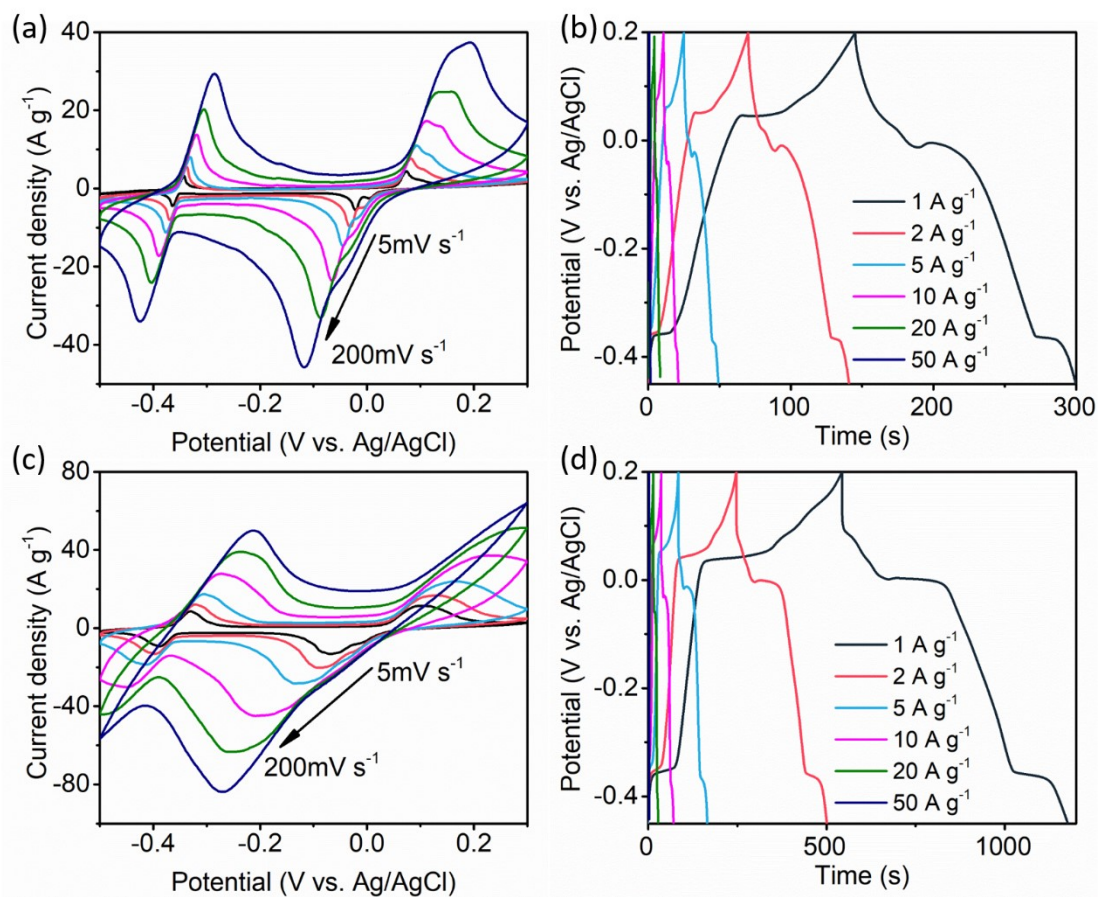


Fig. S8 CV curves of (a) MoO₃ and (c) P0-MoO₃. GCD curves of (b) MoO₃ and (d) P0-MoO₃.

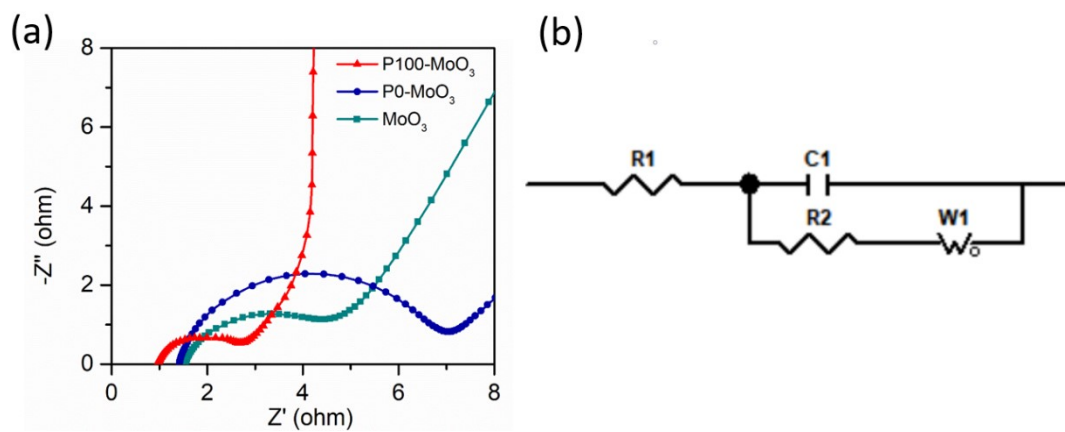


Fig. S9 (a) Magnified high frequency region of the Nyquist plot. (b) Equivalent circuit for the fitting of P100-MoO₃ EIS spectrum.

Table S1 Resistance and hydrogen-ion diffusion coefficient (D_{H^+}) of MoO₃, P0-MoO₃, and P100-MoO₃ fitting/calculated from the EIS spectra.

Materials	R_s (Ω)	R_{ct} (Ω)	R_w (Ω)	D_{H^+} ($\text{cm}^2 \text{s}^{-1}$)
MoO ₃	1.622	1.833	4.038	2.62×10^{-12}
P0-MoO ₃	1.503	4.114	3.853	5.93×10^{-12}
P100-MoO ₃	1.01	1.077	1.924	1.88×10^{-10}

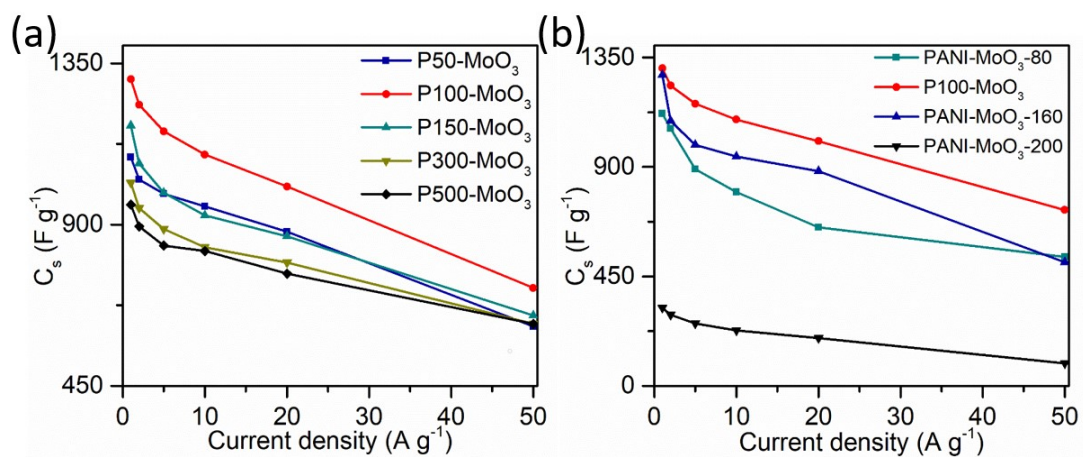


Fig. S10 The compared specific capacitance with different (a) amount of aniline monomers, and (b) hydrothermal temperatures.

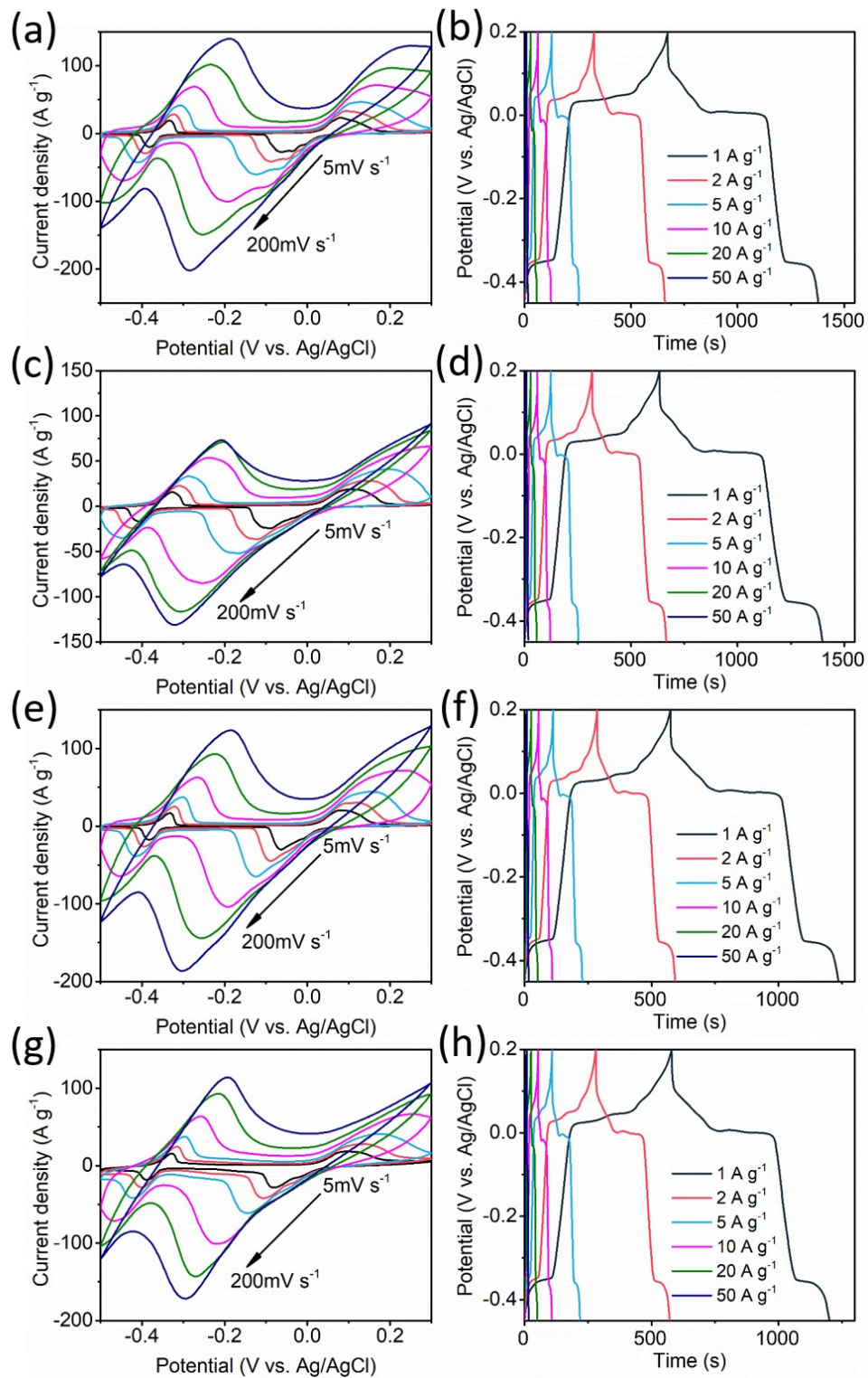


Fig. S11 CV curves of (a) P50- MoO_3 , (c) P150- MoO_3 , (e) P300- MoO_3 and (g) P500- MoO_3 . GCD curves of (b) P50- MoO_3 , (d) P150- MoO_3 , (f) P300- MoO_3 and (h) P500- MoO_3 .

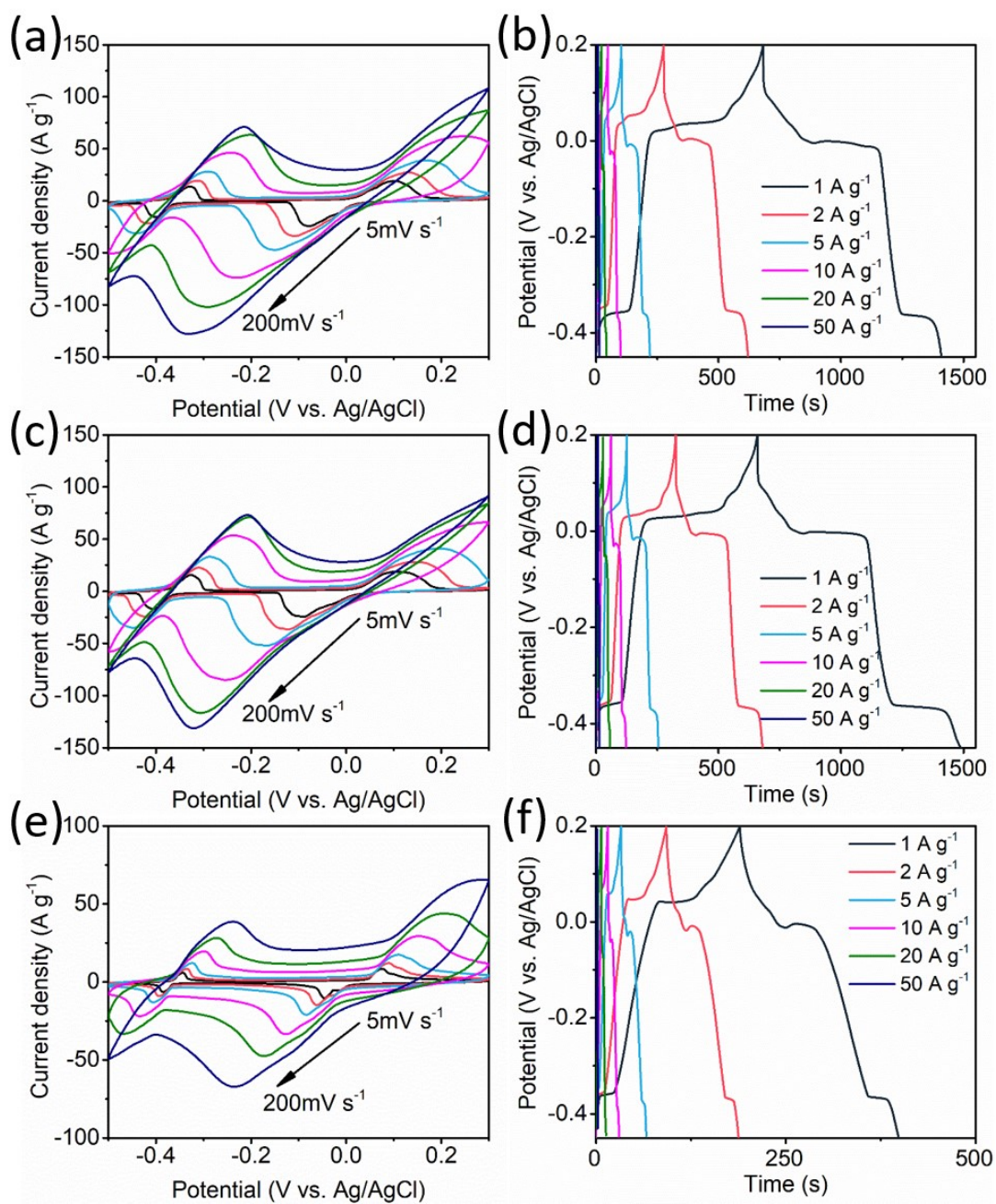


Fig. S12 CV curves of (a) PANI-MoO₃-80, (c) PANI-MoO₃-160 and (e) PANI-MoO₃-200. GCD curves of (b) PANI-MoO₃-80, (d) PANI-MoO₃-160 and (f) PANI-MoO₃-200.

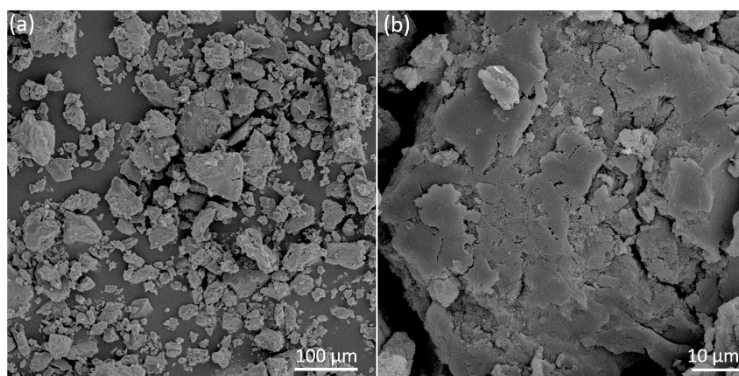


Fig. S13 The SEM images of PANI.

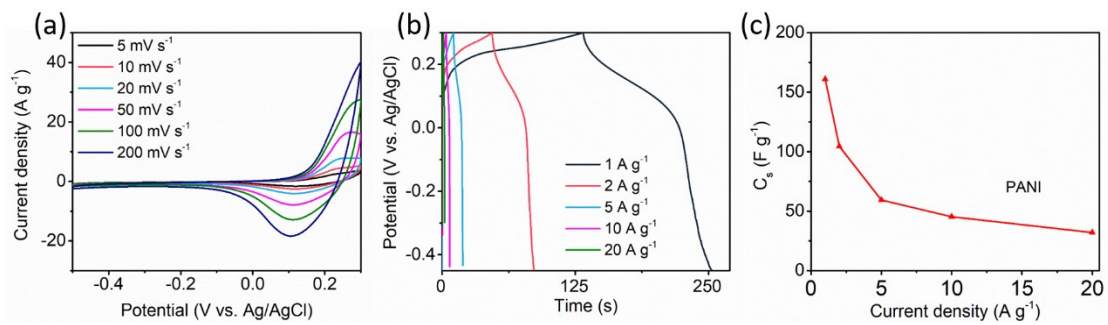


Fig. S14 (a) CV curves, (b) GCD curves, and (c) specific capacitance of pristine PANI.

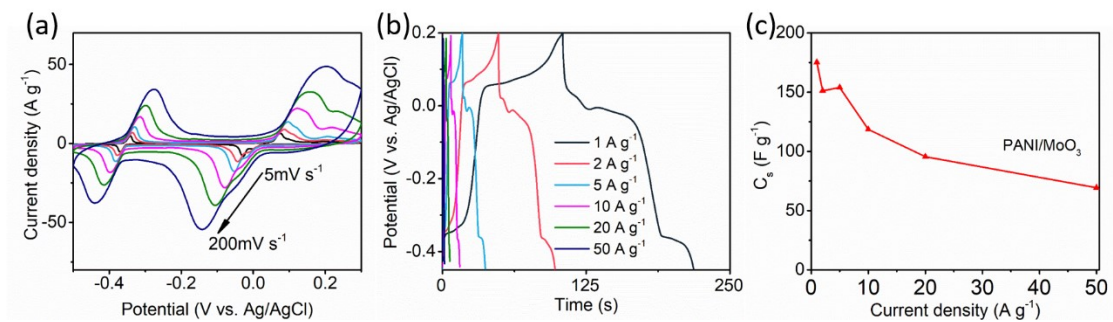


Fig. S15 (a) CV curves, (b) GCD curves and (c) specific capacitance of physical mixture of PANI and commercial MoO_3 .

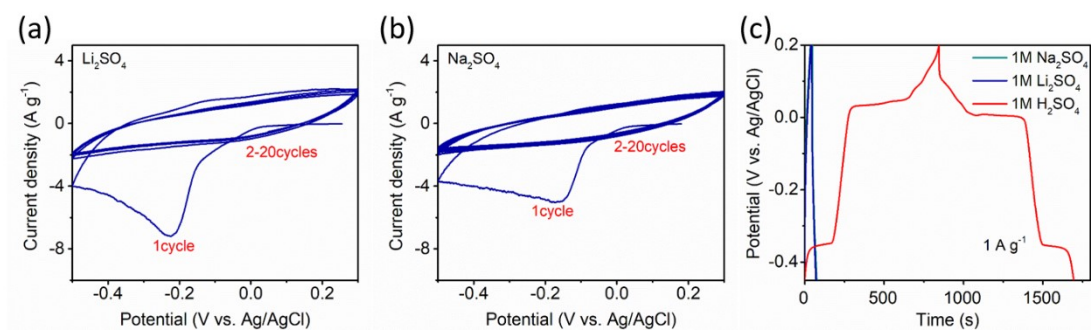


Fig. S16 The CV curves of P100-MoO₃ at the first 20 cycles at electrolyte of (a) 1 M Li₂SO₄, (b) 1M Na₂SO₄ and (c) the GCD curves of P100-MoO₃ in different electrolytes.

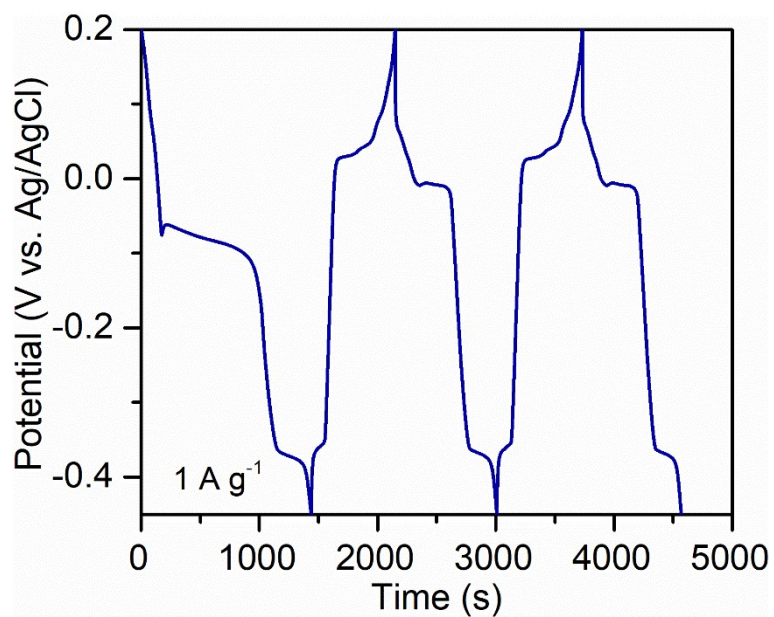


Fig. S17 The charge/discharge curves of the first three cycles of P100-MoO₃ electrode at the current density of 1 A g⁻¹.

The number of hydrogen ions (n) as charge carriers was calculated based on the following formula:

$$n = \frac{C_s \times m \times v}{F}$$

Where C_s is the specific capacitance (F g⁻¹), F is the Faraday constant (96,485 C mol⁻¹), m is the molecular weight and v is the redox potential window.

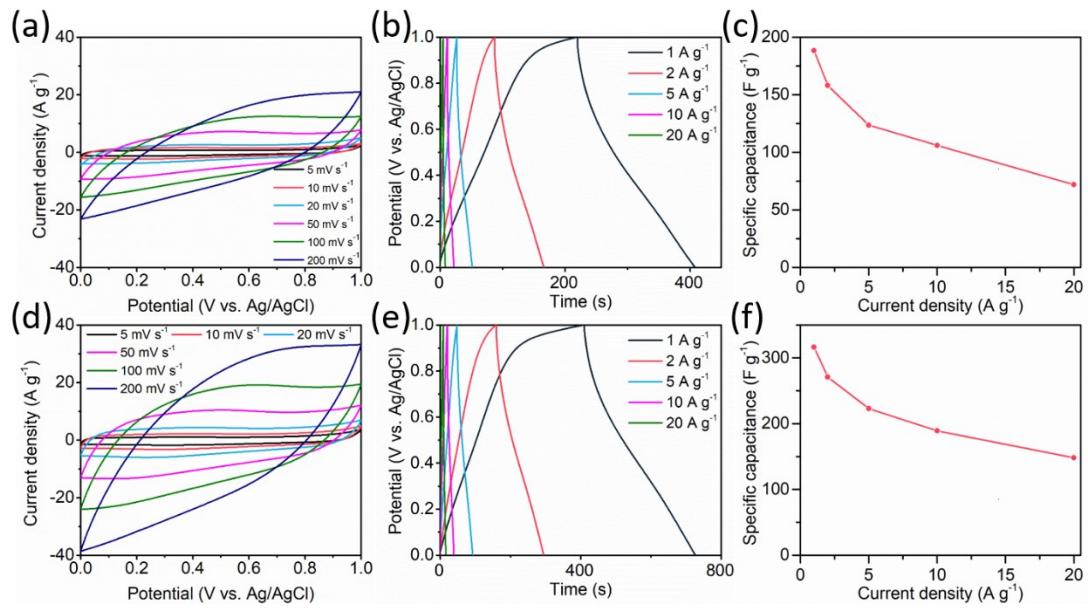


Fig. S18 (a) CV curves, (b) GCD curves, and (c) specific capacitance of AC electrode.

(d) CV curves, (e) GCD curves, and (f) specific capacitance of NAC electrode.

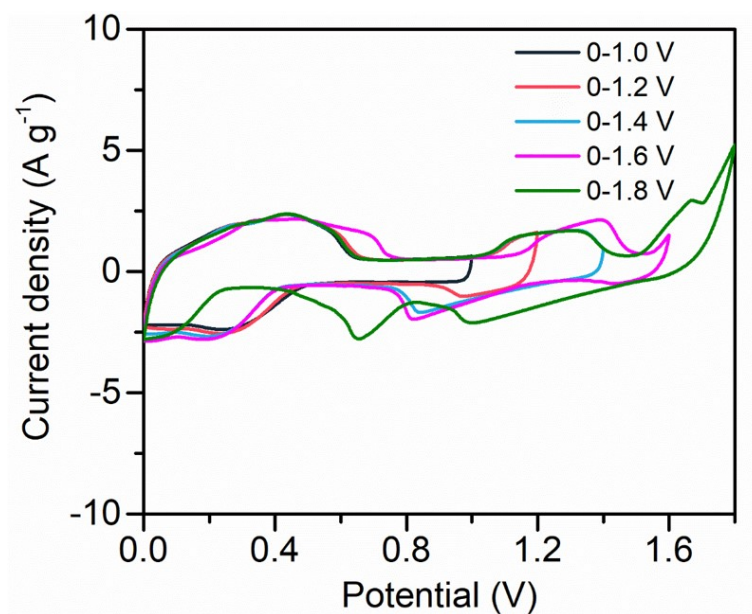


Fig. S19 The CV curves of P100-MoO₃//NAC PBSH device at different potential windows.

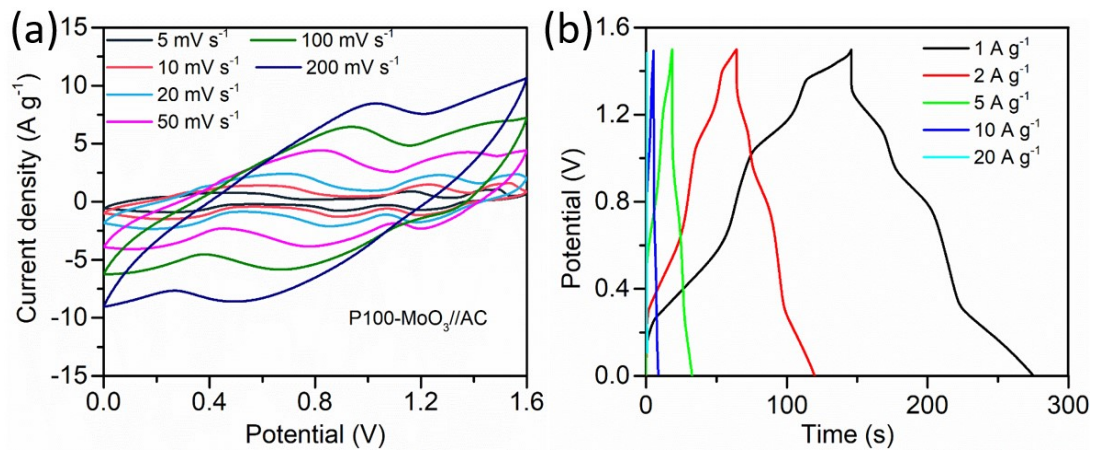


Fig. S20 The P100-MoO₃//AC PBSH device of (a) CV curves and (b) GCD curves.