Supporting Information for

A “one-for-three” Strategy through a Facile One-step Hydrothermal Engineering of Commercial MoO$_3$ for High-Performance Proton Storage

Weifeng Liu,$^a$ Zhi Zhang,*$^a$ Junjie Shi,$^a$ Yifan Zheng,$^a$ Yonghui Wu,$^a$ Xiutao Fu,$^a$ Nishuang Liu,$^a$ Jun Su$^a$
and Yihua Gao$^a$

$^a$ School of Physics & Wuhan National Laboratory for Optoelectronics (WNLO), Huazhong University of Science and Technology (HUST), Luoyu Road 1037, Wuhan 430074, P. R. China.

E-mail: zzhang@hust.edu.cn
Calculation of specific gravimetric capacitance, energy density and power density

The specific of gravimetric capacitance are determined by the following calculation formulas:

\[ C_s = \frac{I \times \Delta t}{m \times \Delta V} \]  \hspace{1cm} (1)

Where \( C_s \) (\( F \text{ g}^{-1} \)) is the specific gravimetric capacitance, \( I \) (A) is the discharge current, \( \Delta t \) (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:

\[ E = \frac{1}{2 \times 3.6} C_s \Delta V^2 \]  \hspace{1cm} (2)
\[ P = \frac{3600 \times E}{\Delta t} \]  \hspace{1cm} (3)

\( E \) (\( Wh \text{ kg}^{-1} \)) and \( P \) (\( W \text{ kg}^{-1} \)) are the energy density and power density, respectively.
**Fig. S1** (a, b) SEM images of P0-MoO$_3$ at different magnifications.
Fig. S2 SEM images of (a) P50-MoO\textsubscript{3}, (b) P150-MoO\textsubscript{3}, (c) P300-MoO\textsubscript{3}, and (d) P500-MoO\textsubscript{3}.
Fig. S3 SEM images of (a) PANI-MoO$_3$-80, (b) P100-MoO$_3$, (c) PANI-MoO$_3$-160, and (d) PANI-MoO$_3$-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-MoO$_3$ showing the Mo 3p and N1s.
Fig. S7 Thermogravimetric analysis (TGA) of pristine MoO$_3$ and P100-MoO$_3$. 
Fig. S8 CV curves of (a) MoO$_3$ and (c) P0-MoO$_3$. GCD curves of (b) MoO$_3$ and (d) P0-MoO$_3$. 
Fig. S9 (a) Magnified high frequency region of the Nyquist plot. (b) Equivalent circuit for the fitting of P100-MoO$_3$ EIS spectrum.
Table S1  Resistance and hydrogen-ion diffusion coefficient ($D_{H^+}$) of MoO$_3$, P0-MoO$_3$, and P100-MoO$_3$ fitting/calculated from the EIS spectra.

<table>
<thead>
<tr>
<th>Materials</th>
<th>$R_s$ (Ω)</th>
<th>$R_{ct}$ (Ω)</th>
<th>$R_w$ (Ω)</th>
<th>$D_{H^+}$ (cm$^2$ s$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>MoO$_3$</td>
<td>1.622</td>
<td>1.833</td>
<td>4.038</td>
<td>$2.62 \times 10^{-12}$</td>
</tr>
<tr>
<td>P0-MoO$_3$</td>
<td>1.503</td>
<td>4.114</td>
<td>3.853</td>
<td>$5.93 \times 10^{-12}$</td>
</tr>
<tr>
<td>P100-MoO$_3$</td>
<td>1.01</td>
<td>1.077</td>
<td>1.924</td>
<td>$1.88 \times 10^{-10}$</td>
</tr>
</tbody>
</table>
**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-MoO$_3$-80, (c) PANI-MoO$_3$-160 and (e) PANI-MoO$_3$-200. GCD curves of (b) PANI-MoO$_3$-80, (d) PANI-MoO$_3$-160 and (f) PANI-MoO$_3$-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-MoO$_3$ at the first 20 cycles at electrolyte of (a) 1 M Li$_2$SO$_4$, (b) 1M Na$_2$SO$_4$ and (c) the GCD curves of P100-MoO$_3$ in different electrolytes.
Fig. S17 The charge/discharge curves of the first three cycles of P100-MoO$_3$ 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:

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

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 $\nu$ 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 PSH device at different potential windows.
Fig. S20 The P100-MoO$_3$/AC PBSH device of (a) CV curves and (b) GCD curves.