

Supporting Information

Super-reductive mesoporous phosphomolybdate with high crystallinity and its excellent performance for Li-ion battery application

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Figure S1. The low-angle XRD pattern of mPMA.

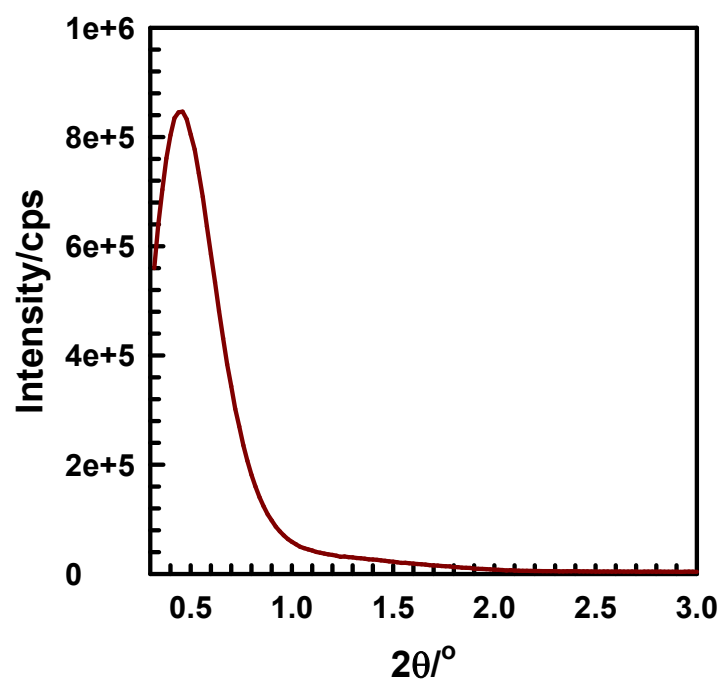


Figure S2. The pore size distribution curve of mPMA.

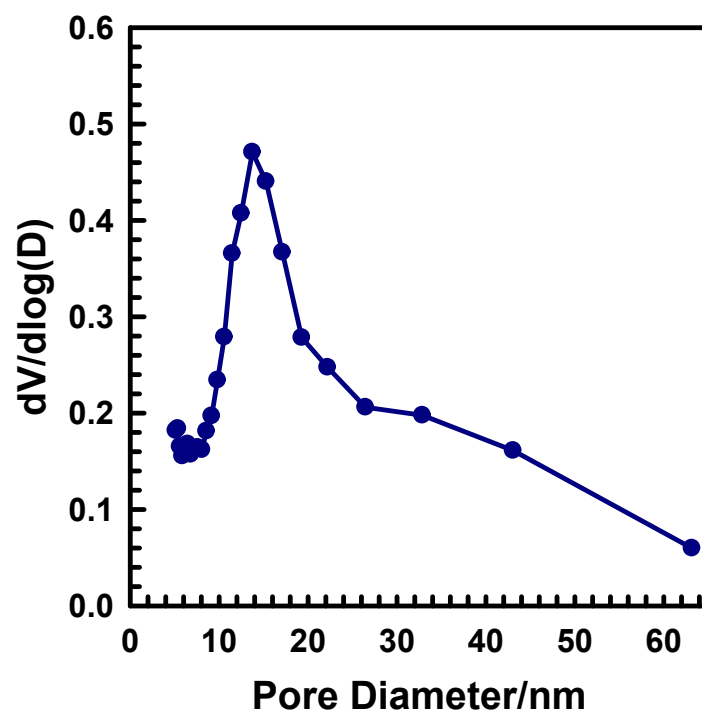
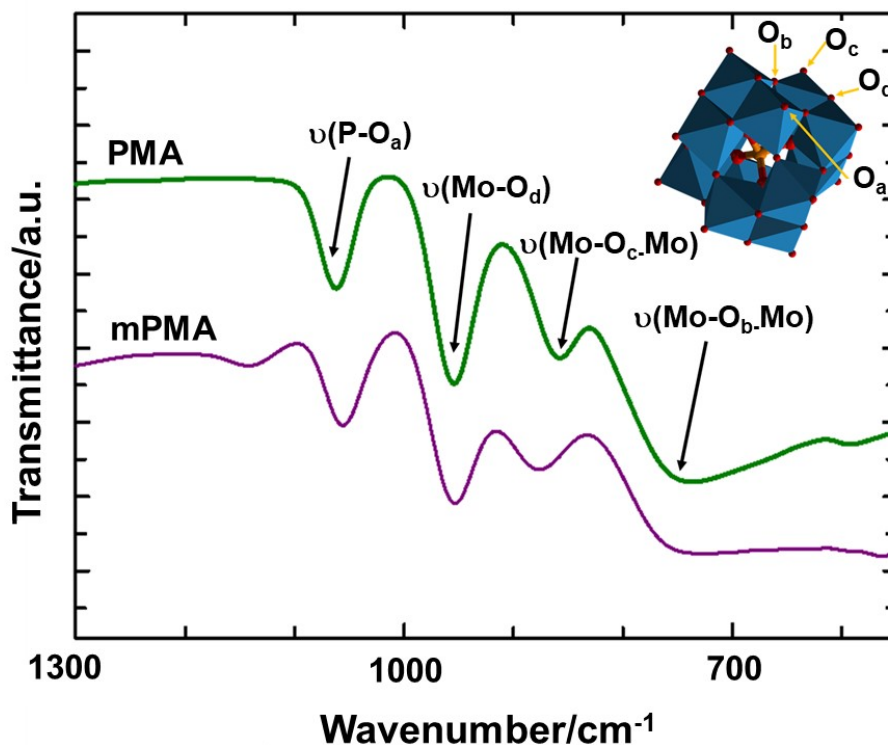


Figure S3. FTIR spectroscopy of mPMA and bulk PMA.



The chemical bonding of mPMA was investigated by Fourier transform-infrared (FT-IR) spectroscopy. The bulk PMA shows the characteristic absorption bands at ~ 770 , ~ 859 , ~ 955 and $\sim 1061 \text{ cm}^{-1}$, which can be assigned to the stretching modes of edge-sharing $\text{Mo-O}_b\text{-Mo}$ and corner-sharing $\text{Mo-O}_c\text{-Mo}$ in MoO_6 octahedra, terminal Mo-O_d bonds and P-O_a bonds in PO_4 tetrahedron respectively. The absorption peaks at $\sim 1050 \text{ cm}^{-1}$ and $\sim 593 \text{ cm}^{-1}$ are assigned to the P-O stretching mode of distorted PO_4 central unit and the stretching vibration mode of O-P-O bonds, respectively. In addition mPMA, shows a slight band below 1200 cm^{-1} compared to bulk PMA, this also demonstrates the PMA clusters are trapped within the mesochanneled formed by keggin anion and potassium ion but they have retained their inherent structure. The mPMA

samples exhibit a shift of the Mo-O_d and Mo-O_b-Mo absorption bands to lower wavenumber region, confirming strongly bonded Keggin anions within the mesostructure.

Figure S4. P 2p high resolution XPS spectra of mPMA and bulk PMA.

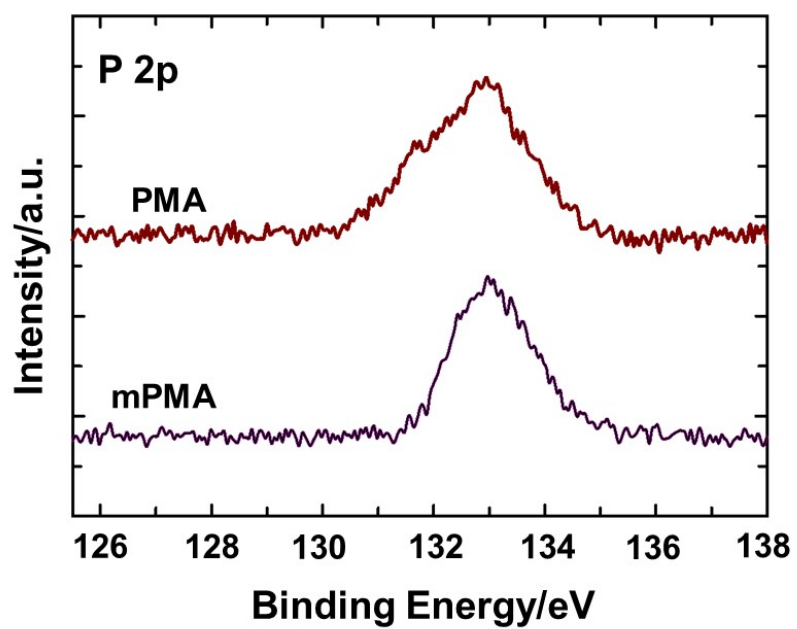


Figure S5. Thermal gravimetric analysis for mPMA and bulk PMA.

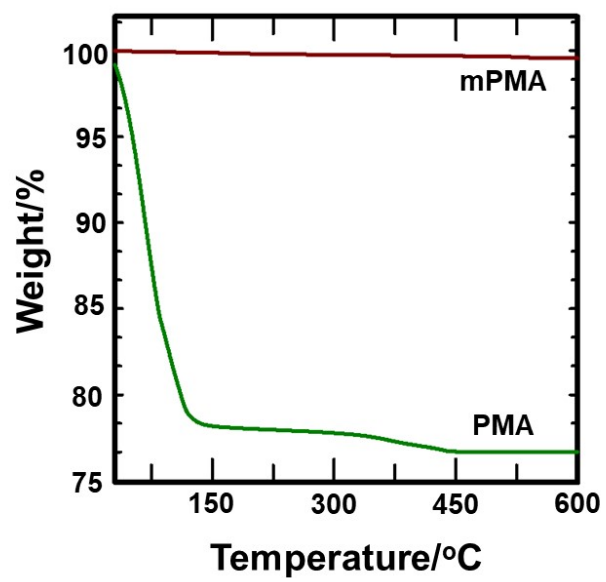


Figure S6. galvanostatic charge-discharge potential profiles at different current densities for the mPMA anode.

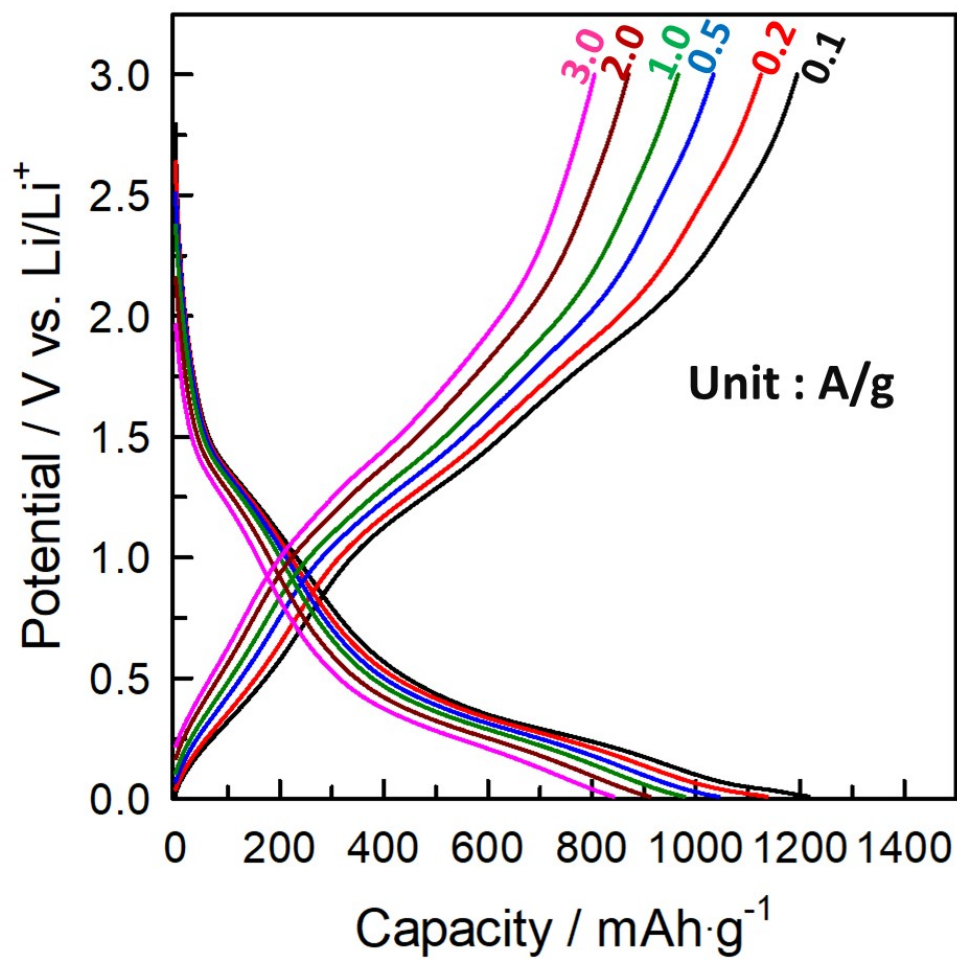


Figure S7. *Ex situ* XRD of mPMA electrode at four different voltages in the initial cycling, where the electrode discharges until 1.5 V (red) and 0.01 V (green) and then charges to ~ 1.5 V (blue) and 3.0 V (pink). Triangles represent the Bragg reflections corresponding to mPMA structure.

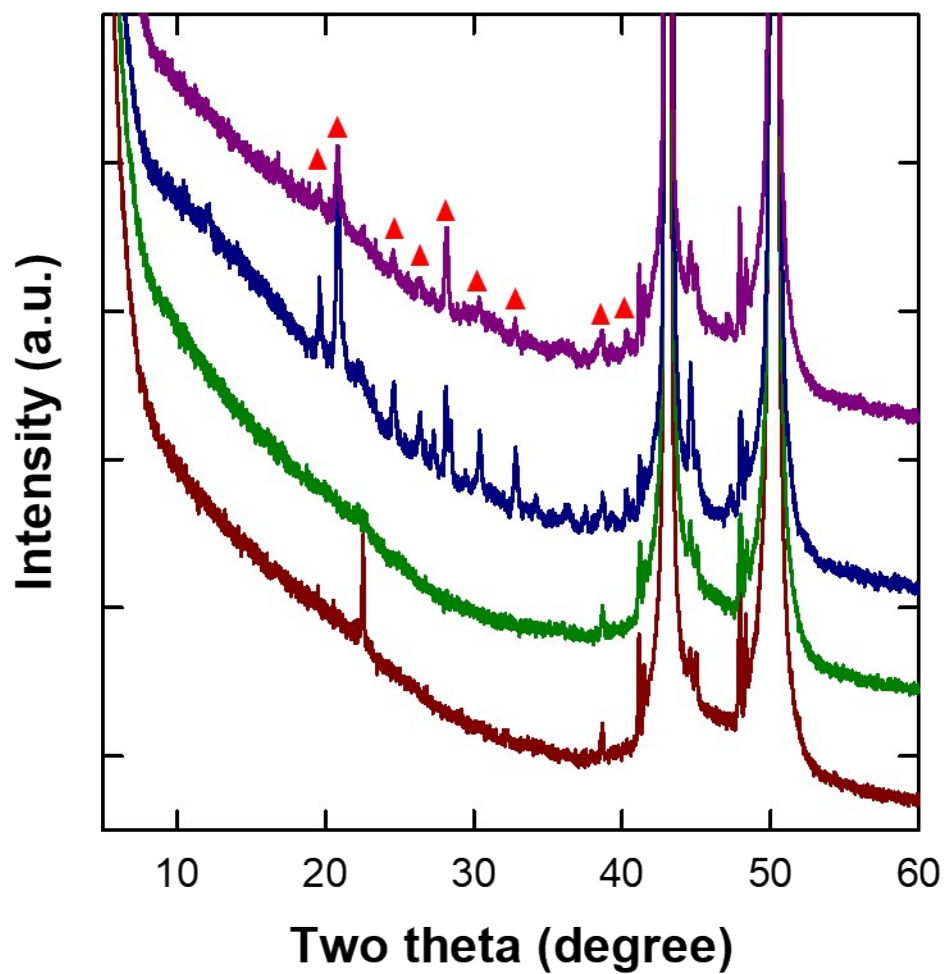


Figure S8. (a) Potential profiles, (b) charge-discharge capacities with Coulombic efficiency at 0.2 Ag^{-1} and (c) rate capability under different current densities of **PMA**

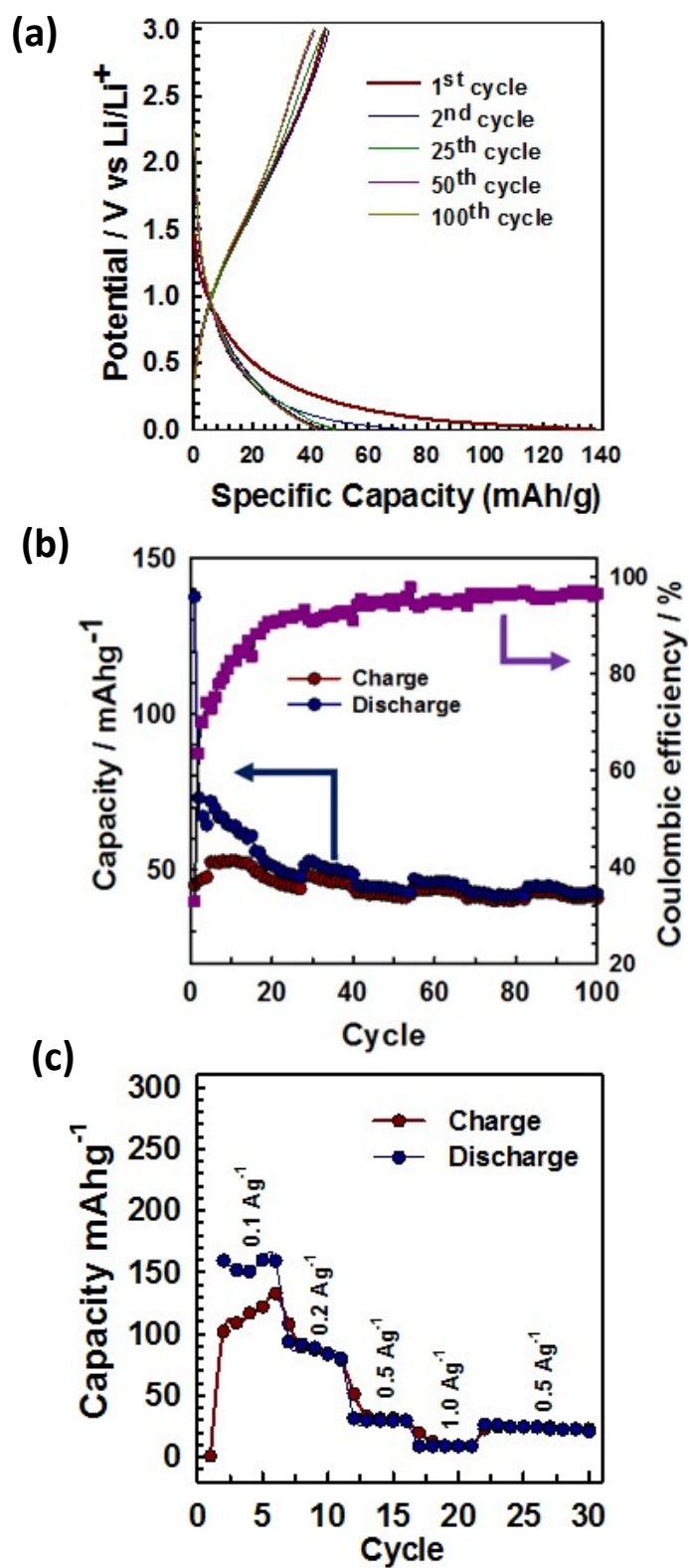


Figure S9. GITT curves of **mPMA** (a) first discharging profile, (b) charging profile and its corresponding estimated Li^+ diffusion coefficients (c) and (d).

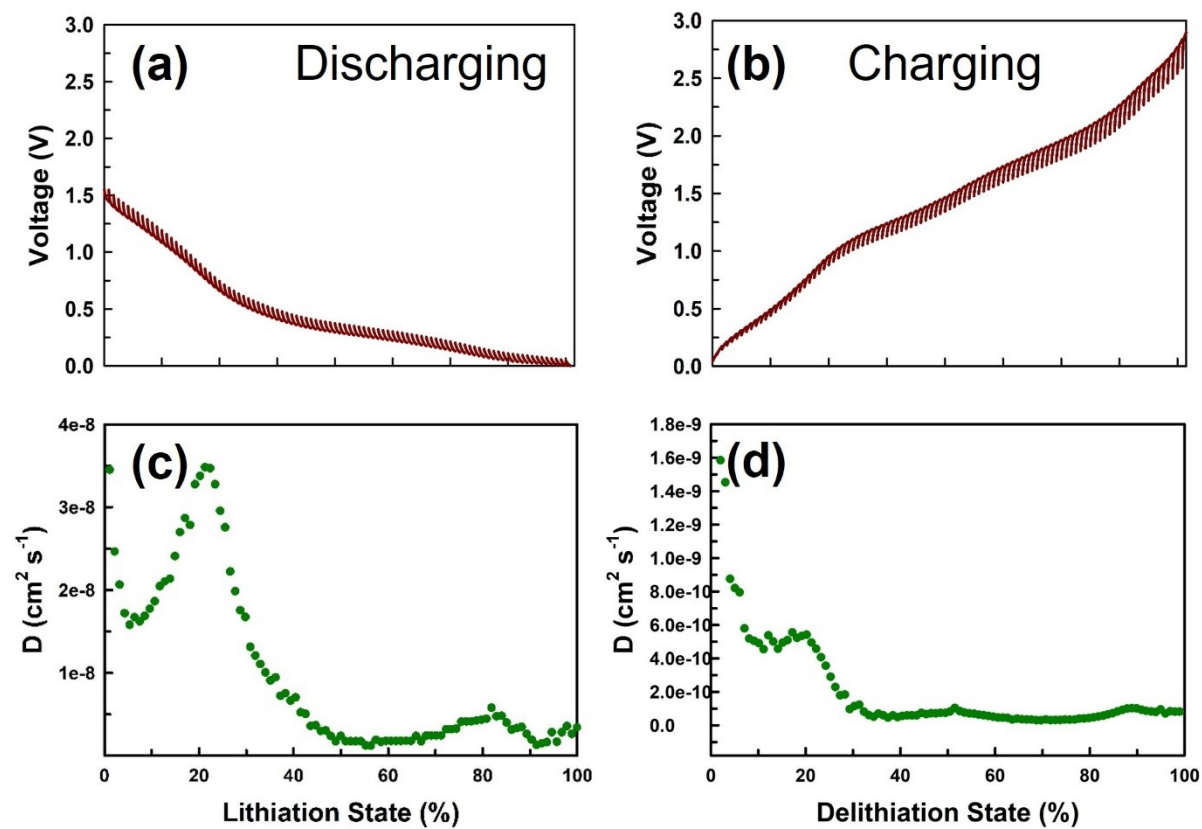


Table S1. Comparison of electrode performances of molybdenum oxide-based materials for LIBs.

Material	Current density	Voltage window (V)	Discharge capacity (mA h g ⁻¹)	Ref.
MoO ₂ /C	200 mA g ⁻¹	0.005-3.0	810	1
MoOC/MoO ₂ -NCNW	500 mA g ⁻¹	0.05-3.0	860	2
Hollow MoO ₂ /C	1000 mA g ⁻¹	0.01-3.0	810	3
MoO _{3-x} nanowire	200 mA g ⁻¹	0.1-3.5	580	4
Mixed molybdenum Oxides	200 mA g ⁻¹	0.005-3.0	930.6	5
Vanadium oxide/ molybdenum oxide hybrid	200 mA g ⁻¹	0.01-3.0	1380	6
Molybdenum oxide Nanobelt	500 mA g ⁻¹	0.01-3.0	291	7
Mesoporous PMA	500 mA g⁻¹	0.01-3.0	1517	This work

Table S2. Comparison of performances of high performing and durable electrode materials for LIBs.

Material	Current density	Voltage window (V)	Discharge capacity (mA h g ⁻¹)	No. cycles	Ref.
Fe ₂ O ₃ /TiO ₂	0.5 A g ⁻¹	0.01-1.0	1056	1000	8
Hollow SnO ₂ -C hybrid nanoparticles	0.5 A g ⁻¹	0.01-3.0	995	500	9
HfO ₂ coated SnO ₂ /MXene	0.5 A g ⁻¹	0.01-3.0	843	50	10
Carbon-Encapsulated Nb ₂ O ₅ Nanocrystals	1.0 A g ⁻¹	0.01-3.0	150	1000	11
NiS _x @C yolk-shell	1.0 A g ⁻¹	0.01-3.0	460	2000	12
CuGeO ₃ ultrathin nanosheets/graphene	1.0 A g ⁻¹	0.01-3.0	693	500	13
SnO ₂ @MOF	1.0 A g ⁻¹	0.01-3.0	450	1000	14
H-TiO ₂ @SnS ₂ @PPy	2.0 A g ⁻¹	0.01-3.0	508	2000	15
Graphene encapsulated ZnO-Mn-C hollow microspheres	5.0 A g ⁻¹	0.01-3.0	422	1600	16
Mesoporous PMA	0.5 Ag⁻¹	0.01-3.0	1517	200	This work
	5.0 A g⁻¹	0.01-3.0	521	500	
Al@TiO ₂ yolk-shell	10 C ⁺	0.06-2.0	661	500	17
Three-dimensional holey-graphene/niobia	10 C [*]	1.1-3.0	125	10000	18

⁺ 1 C=1410 mA g⁻¹

^{*} 10 C= 22 mA cm⁻²

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