

Supporting Information

Micro-Sized MoS₆@15%Li₇P₃S₁₁ Composite Enables Stable All-Solid-State Battery with High Capacity

Mingyuan Chang^{1,2,3}, Mengli Yang¹, Wenrui Xie¹, Fuli Tian¹, Gaozhan Liu¹,

Ping Cui^{1,4}, Tao Wu^{2,3,5}, Xiayin Yao^{1,4*}*

¹ Ningbo Institute of Materials Technology and Engineering, Chinese Academy of Sciences, Ningbo 315201, P.R. China

² Municipal Key Laboratory of Clean Energy Technologies of Ningbo, University of Nottingham Ningbo China, Ningbo 315100, China

³ Department of Chemical and Environmental Engineering, University of Nottingham Ningbo China, Ningbo 315100, China

⁴ Center of Materials Science and Optoelectronics Engineering, University of Chinese Academy of Sciences, Beijing 100049, P.R. China

⁵ Key Laboratory of Carbonaceous Wastes Processing and Process Intensification of Zhejiang

** Correspondence authors: tao.wu@nottingham.edu.cn; yaoxy@nimte.ac.cn.*

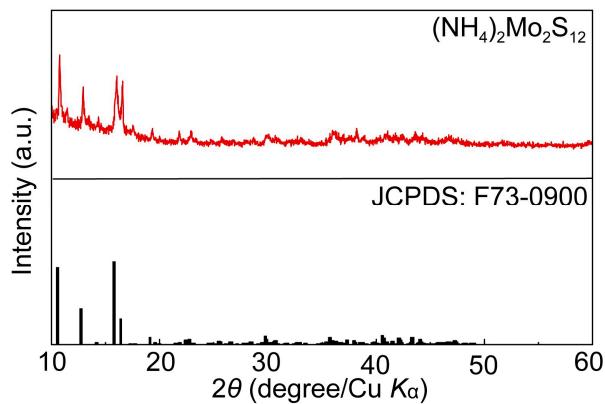


Figure S1. XRD pattern of $(\text{NH}_4)_2\text{Mo}_2\text{S}_{12}$.

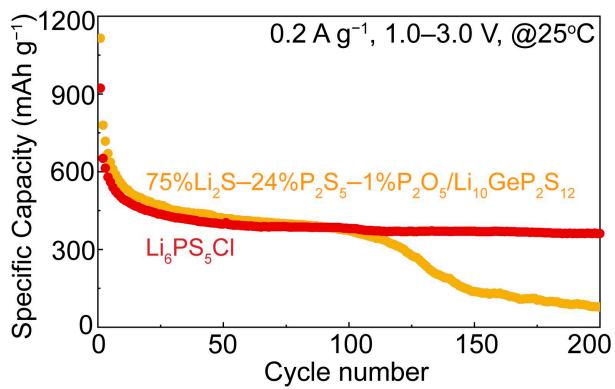


Figure S2. Cyclic performances of Li/Li₆PS₅Cl/MoS₆ and Li/75%Li₂S-24%P₂S₅-1%P₂O₅/Li₁₀GeP₂S₁₂/MoS₆ all-solid-state batteries under 0.2 A g⁻¹.

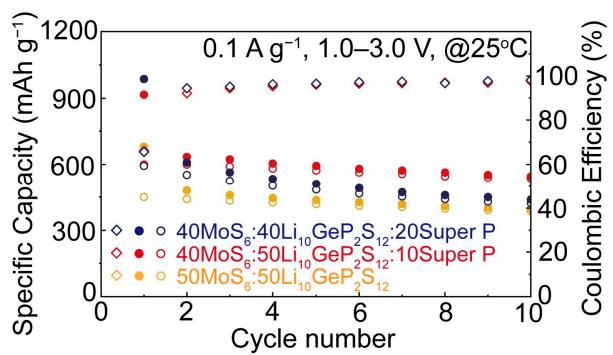


Figure S3. Cyclic performances of all-solid-state batteries with 50MoS₆:50Li₁₀GeP₂S₁₂, 40MoS₆:50Li₁₀GeP₂S₁₂:10Super P and 40MoS₆:40Li₁₀GeP₂S₁₂:20Super P cathodes under 0.1 A g⁻¹.

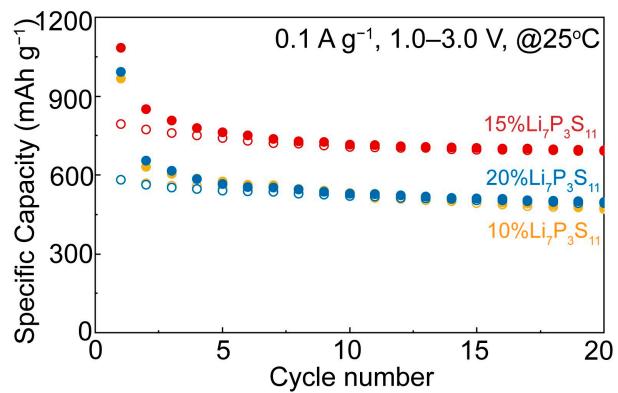


Figure S4. Cyclic performances of MoS₆@10%Li₇P₃S₁₁, MoS₆@15%Li₇P₃S₁₁ and MoS₆@20%Li₇P₃S₁₁ cathodes under 0.1 A g⁻¹.

Table S1. Inductively coupled plasma emission spectrometer analysis of MoS₆.

Elements	S	Mo
Weight %	63.5	31.5
Atom %	85.7	14.2

Table S2. Electrochemical performances comparisons of various active materials in all-solid-state-batteries.

Active Material	Electrolyte	Anode	Voltage Range (V)	Initial Capacity (mAh g ⁻¹)	Reversible Capacity (mAh g ⁻¹)	Reference
rGO-MoS ₃	Li ₁₀ GeP ₂ S ₁₂ /75%Li ₂ S–24%P ₂ S ₅ –1%P ₂ O ₅	Li	0.5–3 V	1241.4	~760	17
Cubic FeS ₂	77.5%Li ₂ S–22.5%P ₂ S ₅	Li	1–3 V	750	~730	10
Co ₉ S ₈ @Li ₇ P ₃ S ₁₁	Li ₁₀ GeP ₂ S ₁₂ /75%Li ₂ S–24%P ₂ S ₅ –1%P ₂ O ₅	Li	0.5–3 V	633	574	21
MoS ₂ @Li ₇ P ₃ S ₁₁	Li ₇ P ₃ S ₁₁	Li	0.1–3 V	868.4	669.2	19
MoS ₆	Li ₆ PS ₅ Cl	Li	1–3 V	913.9	635.1	This work
MoS ₆ @15%Li ₇ P ₃ S ₁₁	Li ₆ PS ₅ Cl	Li	1–3 V	1083.8	851.5	This work

Table S3. EIS fitting results of MoS₆ and MoS₆@15%Li₇P₃S₁₁ under 0.1 A g⁻¹ after 20 cycles.

Cathode materials	1 st cycle		20 th cycle	
	R _e (Ω)	R _{ct} (Ω)	R _e (Ω)	R _{ct} (Ω)
MoS ₆	105.42	/	384.11	52.96
MoS ₆ @15%Li ₇ P ₃ S ₁₁	75.89	/	124.79	10.78

Table S4. MoS₆ values used in energy density and power density calculations.

Current density (A g ⁻¹)	Energy density of active materials (Wh kg ⁻¹)	Energy density of cathode layer (Wh kg ⁻¹)	Time duration (h)	Power density (W kg ⁻¹)
0.1	1209.2	495.8	7.07	70.12
0.2	915.2	375.2	2.66	141.1
0.5	706.2	289.5	0.84	344.7
1.0	559.8	229.5	0.34	675.1
2.0	422.4	173.2	0.13	1332.2

Table S5. MoS₆@15%Li₇P₃S₁₁ composite values used in energy density and power density calculations.

Current density (A g ⁻¹)	Energy density of active materials (Wh kg ⁻¹)	Energy density of cathode layer (Wh kg ⁻¹)	Time duration (h)	Power density (W kg ⁻¹)
0.1	1434.2	588	8.27	71.1
0.2	1160.7	475.9	3.33	142.9
0.5	944	387	0.84	351.9
1.0	794.7	325.8	0.47	693.2
2.0	629.3	258	0.19	1358