

**Defect Engineering of molybdenum disulfide nanosheets boosting super Zn<sup>2+</sup>  
storage from polyaniline intercalation cathode Supporting Information**

Rui Sun, Siyang Dong, Jiekai Yang, Jing Xiong, Caihong Wang, Shengjun Lu\*, Yufei Zhang\* and Haosen Fan\*

*College of Materials Science and Metallurgy Engineering, Guizhou University, Guiyang 550025, China*

E-mail: [hsfan@gzhu.edu.cn](mailto:hsfan@gzhu.edu.cn); [sjlu@gzu.edu.cn](mailto:sjlu@gzu.edu.cn); [hsfan@gzhu.edu.cn](mailto:hsfan@gzhu.edu.cn)

## Experimental section

### Chemicals

Ammonium molybdate and thiourea were purchased from Shanghai Macklin Biochemical Company Limited. Aniline, and isopropanol directly buy from Shanghai Aladdin Bio-Chem Technology Company Limited. The nitric acid comes from Sinopharm Chemical Reagent Company Limited. All chemicals were used as received.

### Synthesis of MoO<sub>3</sub> nanobelts

Typically, 3 g ammonium molybdate was dissolved in 60 mL deionized water with stirring for 20 mins and then adding 15 mL nitric acid to form a transparent solution. The solution was poured to a 100 mL Teflon autoclave and retention 180 °C for 24 h. After the solution cooling to room temperature, the product was obtained via filtration and drying.

### Synthesis of peony-like MoS<sub>2</sub>

685 mg thiourea dissolve in 60 mL deionized water with stirring for 20 mins. And the 100 mg MoO<sub>3</sub> was poured, followed by ultrasonication for 30 mins. Finally, the solution was transferred to a 100 mL Teflon autoclave and retention at 200 °C for 24 h. The resulting product is obtained by filtration and drying.

### Synthesis of peony-like PA-MoS<sub>2</sub>

In brief, 0.3 g MoS<sub>2</sub> was mixed with 30 mL isopropanol by ultrasonication. After stirring for 15 mins, 5 mL aniline was added to the solution to form an even solution with stirring for 30 mins, and then the solution was maintained at 60 °C for 90 mins. Finally, after the solution cooling to room temperature, the product was obtained via filtration and drying at 60 °C.

### Materials characterization

Thermo Scientific K-Alpha was used to observe the structure characterized. Microstructure and the distribution of elements were observed via JEOL JEM-F200 and Talos F200x G2, respectively. X-ray photoelectron spectroscopy (XPS) was performed on the Thermo Scientific K-Alpha Nexsa system.

### Electrochemical measurements

CR-2032 coin consisted of zinc foil, glass fiber membrane, and 3M Zn(CF<sub>3</sub>SO<sub>3</sub>)<sub>2</sub> served as an anode, separator, and electrolyte, respectively. Material, conductive carbon, and polyvinylidene fluoride were mixed with the ratio of 7:2:1 to fabricate the uniform slurry when the 1-methyl-2-pyrrolidinone was used as a solution, which was painted in the carbon paper. And the carbon paper was moved to a blast dryer to move the 1-methyl-2-pyrrolidinone at 60 °C for 12 h. Electrochemistry performances and galvanostatic intermittent titration technique were tested on the NEWARE battery test system with the voltage window of 0.2-1.3 V (vs Zn/Zn<sup>2+</sup>). The electrochemical workstation (CHI660A) was employed to test electrochemical impedance spectroscopy (EIS) and cyclic voltammetry (CV) curves.

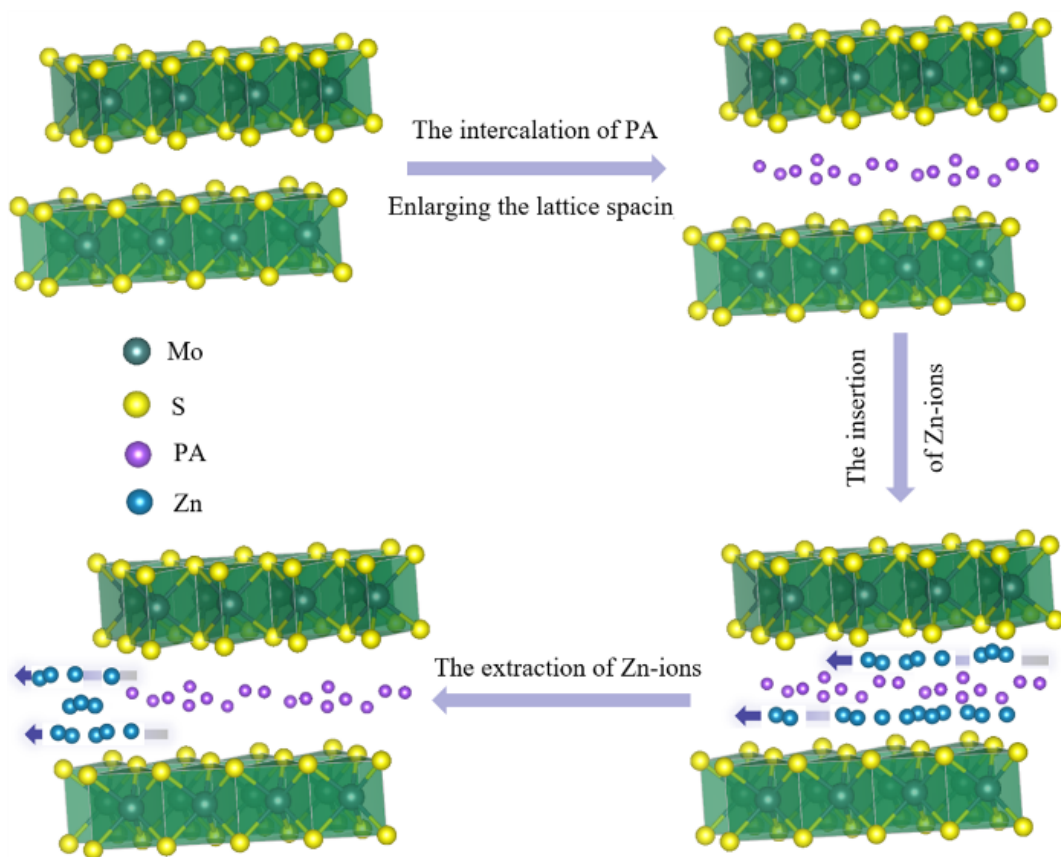


Fig. S1 Schematic illustration of the intercalation/extraction process of Zn-ions during the cycle process.

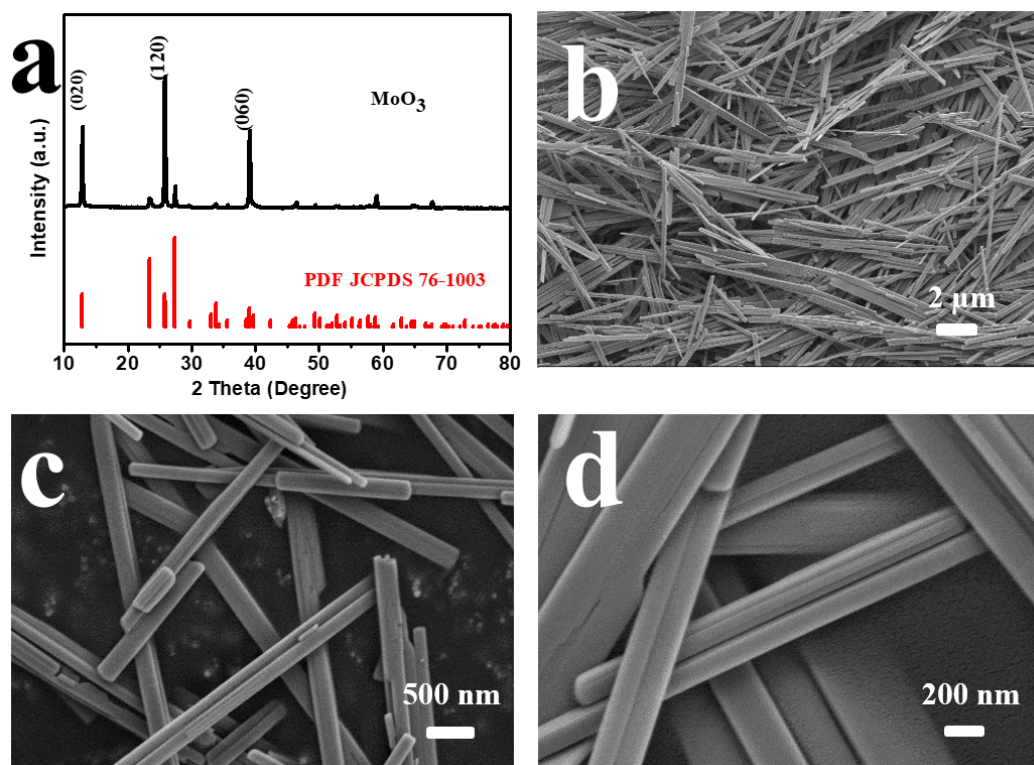


Fig. S2 (a) XRD pattern, (b-c) SEM images of MoO<sub>3</sub>.

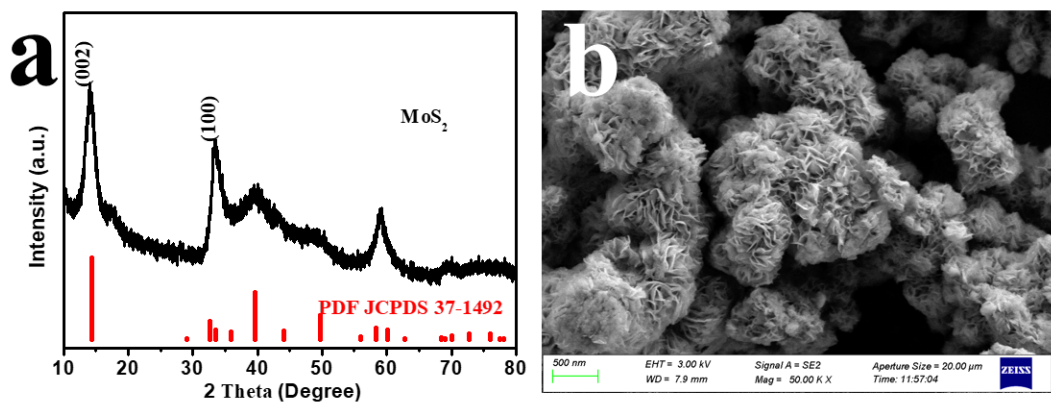


Fig. S3 (a) XRD pattern, (b) SEM images of  $\text{MoS}_2$ .

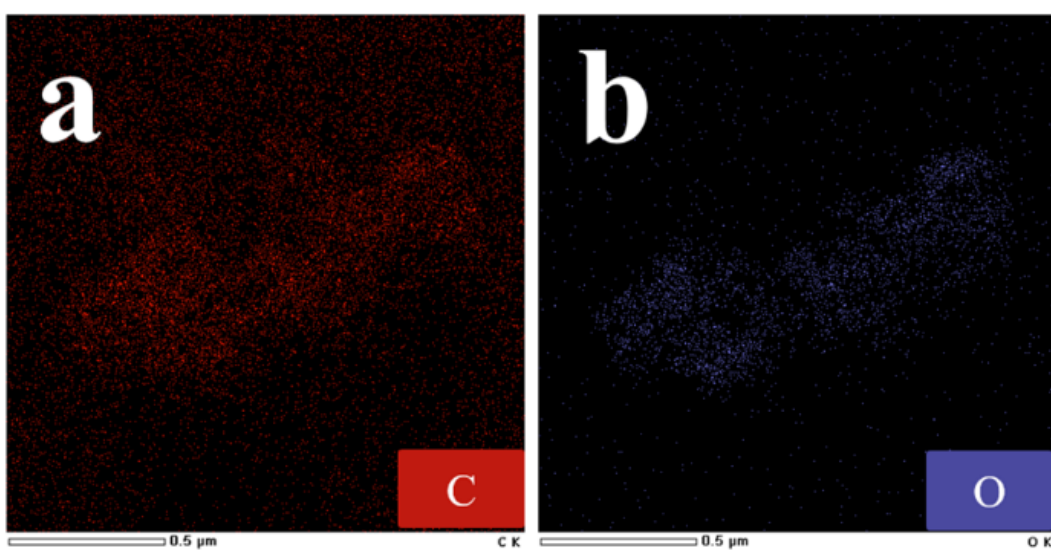


Fig. S4 Elemental mapping of PA- $\text{MoS}_2$ .

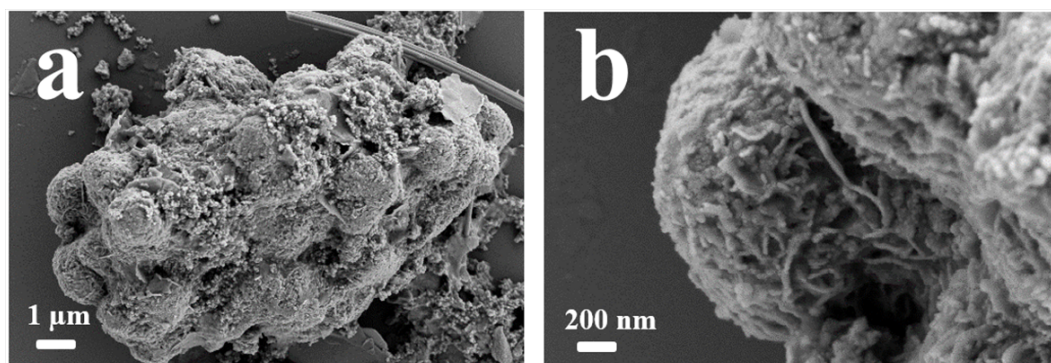


Fig. S6 SEM of PA- $\text{MoS}_2$  after cycling.

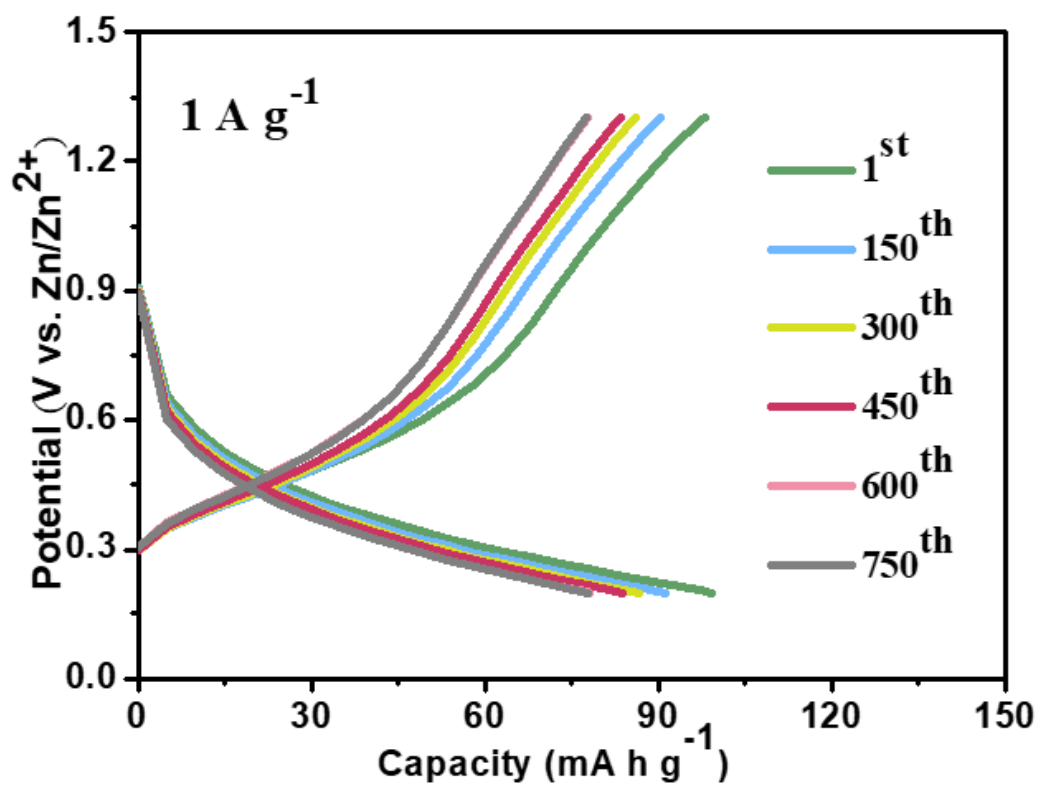


Fig. S7 Galvanostatic charge-discharge curves at  $1 \text{ A g}^{-1}$ .

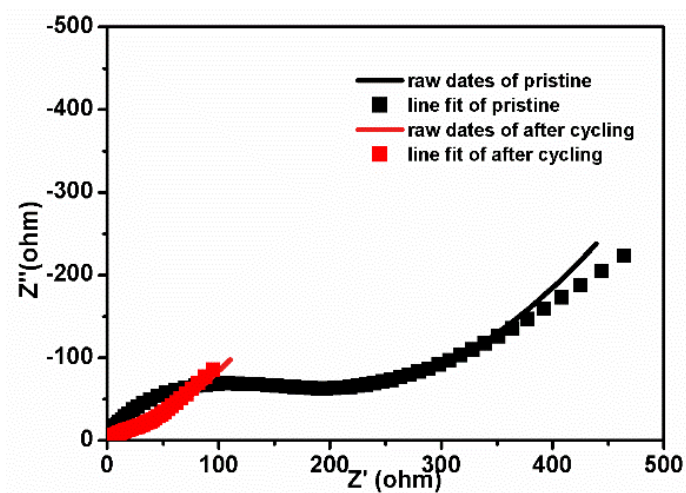


Fig. S7 Nyquist plots of PA-MoS<sub>2</sub>.

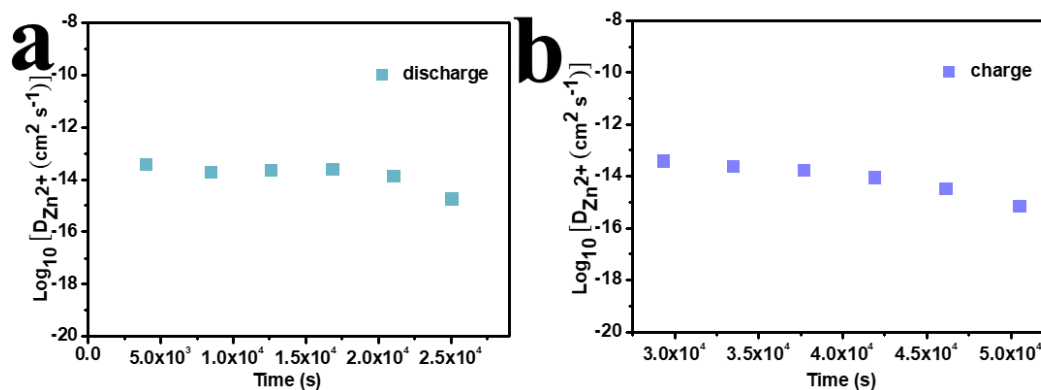


Fig. S8 (a) Zn<sup>2+</sup> diffusion coefficient of the discharge process, (b) the charge process at  $0.1 \text{ A g}^{-1}$ .

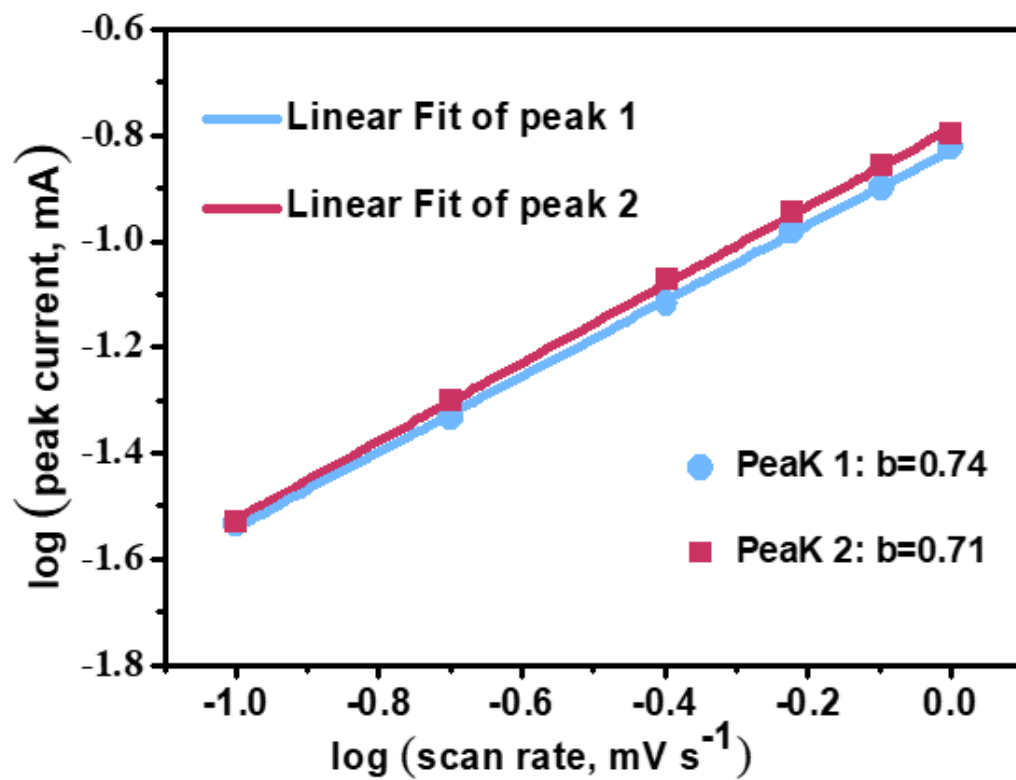


Fig. S9 (a)  $\log(i)$  vs  $\log(mv)$  plots at specific currents.

Table S1. comparison of the electrochemical performance among PA-MoS<sub>2</sub> and other reported Mo-based cathode materials.

Materials	Electrolyte	Voltage window (V vs Zn/Zn <sup>2+</sup> )	Cyclic capacity (mAh g <sup>-1</sup> ) 1/th/A g <sup>-1</sup> )	Ref.
P-MST	3 M Zn(CF <sub>3</sub> SO <sub>3</sub> ) <sub>2</sub>	0.2-1.25	125/100/1; 88/300/2	1
MoS <sub>2</sub> @CNTs	3 M Zn(CF <sub>3</sub> SO <sub>3</sub> ) <sub>2</sub>	0.3-1.2	92.2/500/1	2
TNC@MoS <sub>2</sub> NWS	2 M ZnSO <sub>4</sub>	0.3-1.3	ca. 65/100/0.5	3
MoS <sub>2-x</sub> 250	3 M Zn(CF <sub>3</sub> SO <sub>3</sub> ) <sub>2</sub>	0.25-1.25	92.8/600/0.5	4
<b>PA-MoS<sub>2</sub></b>	<b>3 M Zn(CF<sub>3</sub>SO<sub>3</sub>)<sub>2</sub></b>	<b>0.2-1.3</b>	<b>157.7/80/0.1;</b> <b>77.8/750/1</b>	<b>This work</b>

## References

1. Z. Gan, L. Xia, J. Yin, Y. Gao, X. Feng, G. Meng, Y. Cheng and X. Xu, *ACS Applied Energy Materials*, 2022, **5**, 15452-15462.
2. M. Huang, Y. Mai, L. Zhao, X. Liang, Z. Fang and X. Jie, *ChemElectroChem*, 2020, **7**, 4218-4223.
3. X. Yao, C. Li, R. Xiao, J. Li, H. Yang, J. Deng and M. S. Balogun, *Small*, 2022, **18**, 2204534.
4. W. Xu, C. Sun, K. Zhao, X. Cheng, S. Rawal, Y. Xu and Y. Wang, *Energy Storage Materials*, 2019, **16**, 527-534.