Supporting Information

Enhanced Polysulfides Regulation via Honeycomb-Like Carbon with Catalytic MoC for Lithium-Sulfur Batteries

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Fig. S1. (a) XRD pattern of SiO_2 ; (b) SEM images of SiO_2 .



Fig. S2. SEM images and corresponding elemental mappings of H-MoC-NC.



Fig. S3. TEM images of H-MoC-NC. Blue enclosed region are loosely stacked carbon and orange enclosed region are uniformly distributed MoC.



Fig. S4. SEM and TEM images of MoC.



Fig. S5. XRD pattern of MoC.



Fig. S6. Raman spectrum of H-MoC-NC.



Fig. S7. XPS spectra of H-MoC-NC (a) survey spectra; (b) N 1s; (c) O 1s.

The full range XPS survey spectra involve five distinct peaks of Mo 3d at ~233 eV, C 1s at ~ 285 eV, N 1s at ~ 399 eV, Mo 3p at ~ 417 eV and O 1s at ~ 532 eV. The presence of oxygen element is likely due to the trapped or physically adsorbed oxygen and moisture on the surfaces of samples, or the small amount of oxygen-containing functional group as formed during the synthesis process.



Fig. S8. XRD pattern of S/MoC.



Fig. S9. TGA curve of S/MoC.



Fig. S10. TEM images of the H-MoC-NC after sulfur incorporation.



Fig. S11. (a) XRD pattern of Super P carbon; (b) SEM images of Super P carbon.



Fig. S12. The CV curve of H-MoC-NC as electrode measured in symmetric coin cell using an electrolyte without Li_2S_6 .



Fig. S13. The CV curve of H-MoC-NC as electrode for first three cycles.



Fig. S14. Tafel plots of coin cell derived from peak I, III in CV curves.



Fig. S15. (a) CV curves of S/MoC and (b) S/Super P at different scan rates.



Fig. S16. (a) plot of CV peak current for peaks I, II, and III versus the square root of the scan rates for Super P; (b) for MoC.



Fig. S17. Galvanostatic charge-discharge profiles of (a) MoC; (b) Super P; (c) GCD profiles of different electrodes at a current density of 1 C.



Fig. S18. (a) Enlarged discharge curves of different electrodes at a current density of 0.2 C; (b) charge curves.



Fig. S19. EIS spectrum of the S/H-MoC-NC cathode before and after cycling.



Fig. S20. (a) Charge/discharge curves and (b) cycling stability of pure H-MoC-NC without sulfur content.



Fig. S21. GCD profiles of (a) H-MoC-NC cathode at 3C at different cycles; (b) MoC cathode.



Fig. S22. SEM images of the S/H-MoC-NC cathode structure before and after cycling.



Fig. S23. Energy efficiency of S@/H-MoC-NC compared with S/MoC.



Fig. S24. Digital photo of the LED after lighting for more than half an hour.

Table S1. Comparison of H-MoC-NC electrochemical performance as sulfur host for LSBs

Sulfur hosts	Capacity (low current rate) (mAh/g)	Capacity (high current rate) (mAh/g)	Decay rate (per cycle, %) (times, current rate)	Sulfur loading (%)	Ref
C/Co ₃ O ₄	(0.1C)1036	(3C)428	0.066% (500 cycles, 0.5 C)	66%	1
YSC@Fe ₃ O ₄	(0.1C)1366	(2C)773	0.07% (200 cycles, 0.1C)	80%	2
rod-TiO ₂ @C	(0.2C)1247	(3C)848	0.048%(500 cycles, 0.5C)	65%	3
NiO- NiCo ₂ O ₄ @C	(0.2C)1063	(2C)698	0.059%(500 cycles,0.5C)	73%	4
N- CN@Co ₃ Se ₄	(0.1)1437	(2C)708	0.174%(200 cycles, 0.5C)	61.5%	5
NiCo- LDH@rGO	(0.1C)1336	(2C)713	0.04%(800 cycles, 1C)	73%	6
Ni ₃ (HITP) ₂	(0.1C)1358.6	(2C)696	0.116%(300 cycles, 1C)	65.5%	7
H- TiO _x @S/PPy	(0.1C)1130	(1C)726	0.0406%(1000 cycles, 1C)	69.45%	8
H-MoC-NC	(0.1C)1316	(3 C)646	0.049% (1000 cycles, 3 C)	69.9%	This work

with state-of-the-art cathode materials.

- 1. F. Ma, J. Liang, T. Wang, X. Chen, Y. Fan, B. Hultman, H. Xie, J. Han, G. Wu and Q. Li, *Nanoscale*, 2018, **10**, 5634-5641.
- 2. J. He, L. Luo, Y. Chen and A. Manthiram, *Adv. Mater.*, 2017, **29**, 1702707.
- 3. W. Yao, C. Chu, W. Zheng, L. Zhan and Y. Wang, *Journal of Materials Chemistry A*, 2018, **6**, 18191-18205.
- 4. L. Hu, C. Dai, H. Liu, Y. Li, B. Shen, Y. Chen, S.-J. Bao and M. Xu, *Adv. Energy Mater.*, 2018, **8**, 1800709.
- 5. D. Cai, B. Liu, D. Zhu, D. Chen, M. Lu, J. Cao, Y. Wang, W. Huang, Y. Shao, H. Tu and W. Han, *Adv. Energy Mater.*, 2020, **10**, 1904273.
- 6. W. Qiu, G. Li, D. Luo, Y. Zhang, Y. Zhao, G. Zhou, L. Shui, X. Wang and Z. Chen, *Adv. Sci.*, 2021, **8**, 2003400.
- 7. D. Cai, M. Lu, L. Li, J. Cao, D. Chen, H. Tu, J. Li and W. Han, *Small*, 2019, **15**, 1902605.
- 8. G. Chen, W. Zhong, Y. Li, Q. Deng, X. Ou, Q. Pan, X. Wang, X. Xiong, C. Yang and M. Liu, *ACS Appl. Mater. Interfaces*, 2019, **11**, 5055-5063.

References