

High-conductivity 1T-MoS₂ catalysts anchored on a carbon fiber cloth for high-performance lithium-sulfur batteries

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Table S1. The weight of bare CFC, 2H-MoS₂@CFC, and 1T-MoS₂@CFC

Weight (mg)	1	2	3	4	5	6	Average weight (mg)
Bare CFC	13.89	13.59	13.83	13.75	13.93	13.74	13.79
2H-MoS ₂ @CFC	15.83	15.75	15.87	15.88	15.78	15.67	15.79
1T-MoS ₂ @CFC	15.93	15.82	15.91	15.88	15.80	15.84	15.86

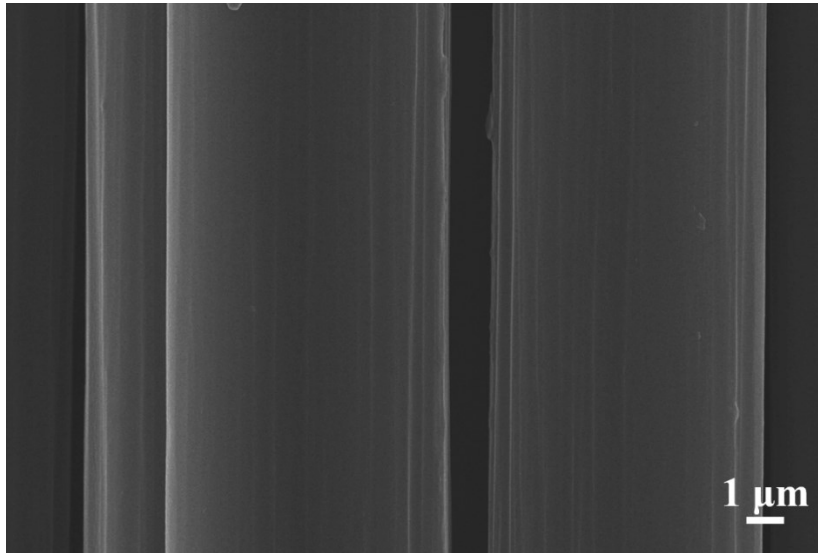


Fig. S1. SEM images of bare CFC.

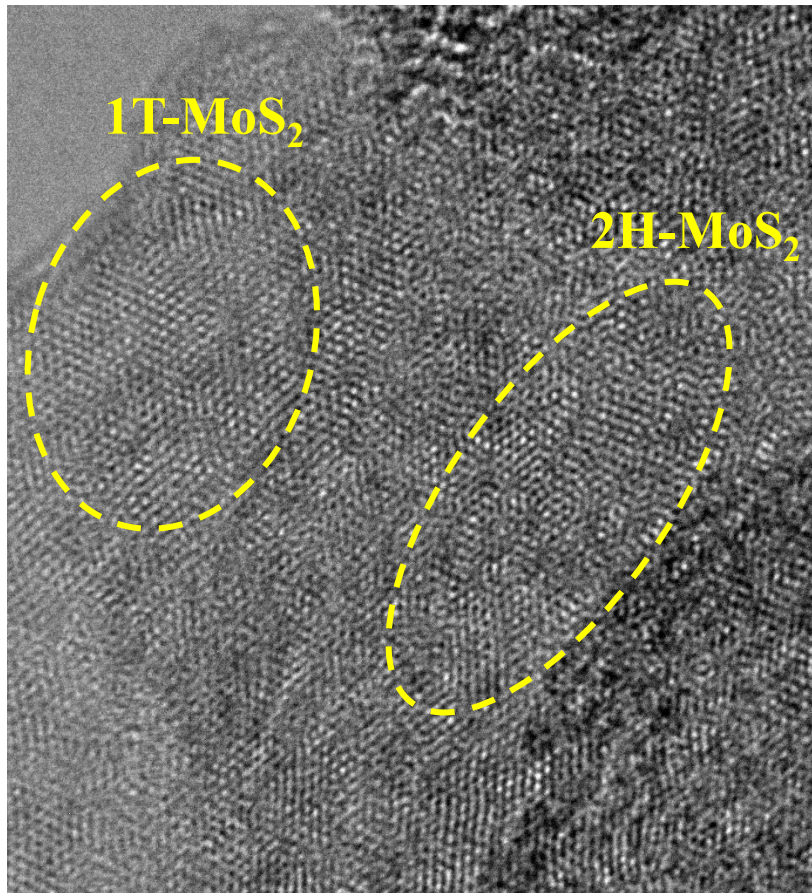


Fig. S2. HTEM images of 1T-MoS₂@CFC.

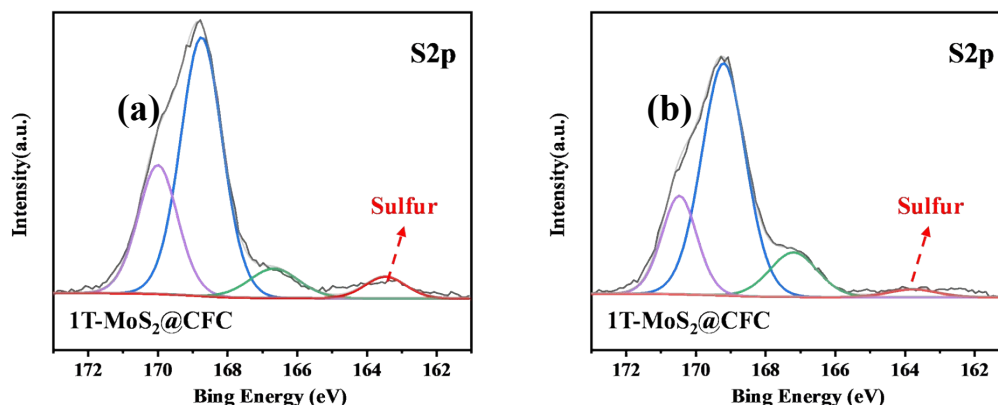


Fig. S3. XPS high-resolution spectra for S 2p of the cathodes taken out from the batteries charged to 2.8V with (a) 2H-MoS₂@CFC and (b) 1T-MoS₂@CFC

The XPS characterization of the cathodes which were charged to 2.8V and were taken out from batteries with 1T-MoS₂@CFC and 2H-MoS₂@CFC, were performed as shown in Fig S3. The peaks during 171eV to 166eV belonged to sulphate species, and the peak at 163.9eV corresponded to elemental sulfur. It was seen that the cathode facing 1T-MoS₂@CFC had more sulfur, indicating that more polysulfides were converted into S, and the reversibility was better. This was due to the fact that the surface and Mo-terminated edges of 1T MoS₂ offered stronger anchor sites for Li₂S, a lower barrier of Li-S decomposition, and faster Li⁺ migration than those for the 2H phase, which demonstrated the unique catalytic property of 1T MoS₂.

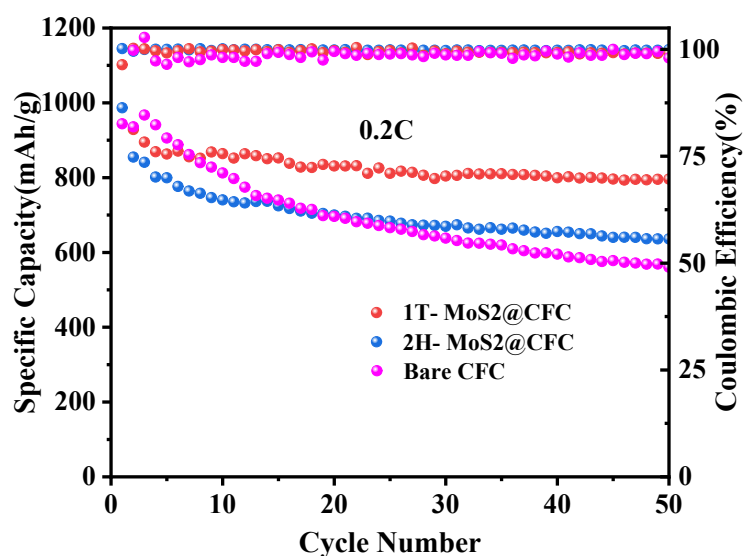


Fig. S4. Cycling performance of the Li-S batteries with Bare CFC, 2H-MoS₂@CFC and 1T-MoS₂@CFC interlayers at 0.2 C.

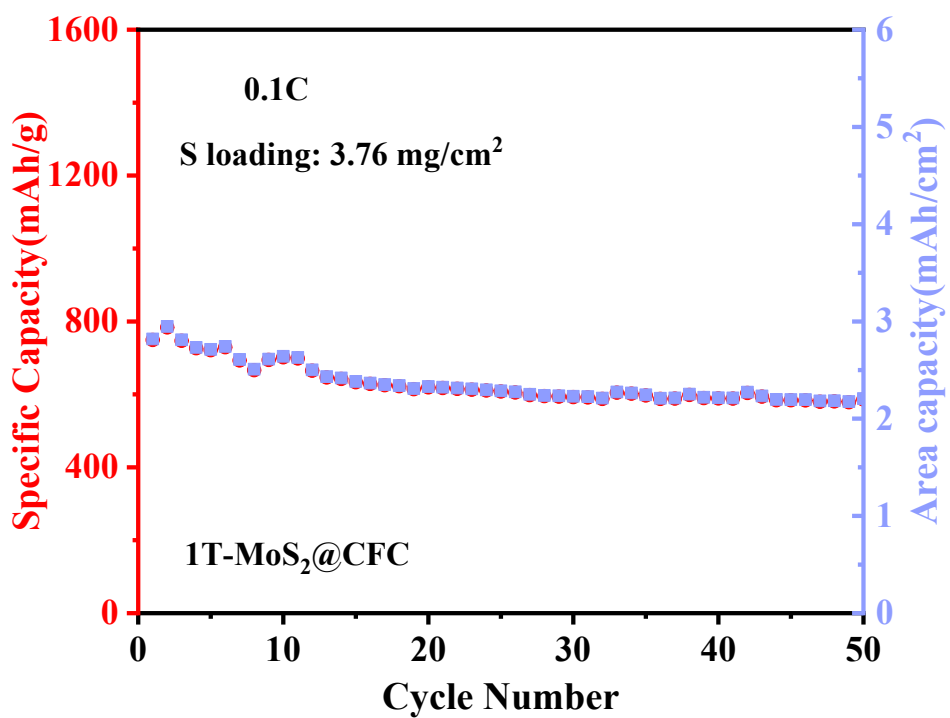


Fig. S5. Cycling performance of the Li-S batteries with 1T-MoS₂@CFC interlayer at a sulfur loading of 3.76mg/cm² at 0.1 C.

Battery with 1T-MoS₂@CFC interlayer still worked normally under high S loading, showing good cycling ability.

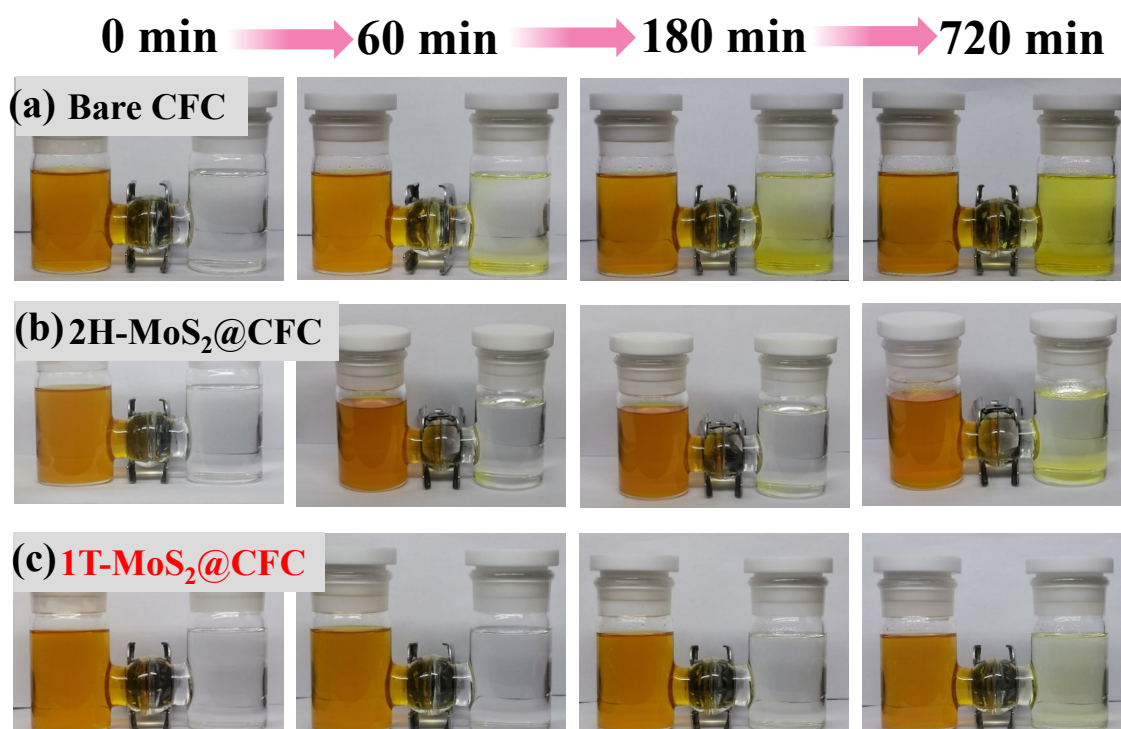


Fig. S6. Permeation test of Li_2S_6 with the (a) Bare CFC, (b) $2\text{H-MoS}_2@\text{CFC}$ (c) $1\text{T-MoS}_2@\text{CFC}$ interlayers.

In this experiment, the left side of the glass shell was the Li_2S_6 solution with a concentration of 0.05 mol L^{-1} , and the right side was the pure DOL solvent. As shown in Fig S6, the lithium polysulfides easily shuttled through the bare CFC interlayer to the right side only after 60 min, and the situation of $2\text{H-MoS}_2@\text{CFC}$ was better, while the other device with the $1\text{T-MoS}_2@\text{CFC}$ modified separator was still colorless. With the increase of time, the color of the device with CFC interlayer and $2\text{H-MoS}_2@\text{CFC}$ interlayer changed to dark yellow and light yellow respectively after 12 h. By contrast, the color of the device with $1\text{T-MoS}_2@\text{CFC}$ slightly changed, indicating that $1\text{T-MoS}_2@\text{CFC}$ effectively suppressed the shuttle effect of polysulfide (Fig S6).

Table S2. Comparison of the electrochemical performance of Li-S batteries with different MoS₂ systems.

Material	Synthesis method /solvent	the role of MoS ₂	Specific initial capacity	Electrochemical performance	Reference
1T-MoS ₂ nanosheets, WS ₂ , rGO	Liquid phase exfoliation /DI	Sulfur host	0.05C, 1140 mAh g ⁻¹	0.5C, 300 cycles, 444.1 mAh g ⁻¹	J. Colloid Interface Sci. 2019 ¹
1T-MoS ₂ nanodots, porous CF	Chemical Li-intercalation/n-butyl lithium solution	Sulfur host	0.1C, 1156 mAh g ⁻¹	0.5C, 300cycles, 620 mAh g ⁻¹	J. Mater. Chem. A, 2020 ²
1T-MoS ₂ nanosheets	Electrochemical exfoliation /DMF	Filter onto separator	0.2C, 1200 mAh g ⁻¹	1C, 500cycles, ~670 mAh g ⁻¹ , CE=95%	J. Mater. Chem. A 2017 ³
2H-MoS ₂ nanosheets, CNTP	Magnetron sputtering way	Self-supporting interlayer	0.5C, 1233 mAh g ⁻¹	0.5C, 100cycles, 850 mAh g ⁻¹	J. Electroanal. Chem. ⁴
2H-MoS ₂ powder	—	Coating separator	0.2C, 1246 mAh g ⁻¹	0.2C, 100 cycles, ~950 mAh g ⁻¹	Ceram. Int. 2019 ⁵
2H-MoS ₂ nanoflowers, GO	Hydrothermal method/DI, annealing treatment	Coating separator	0.2A g ⁻¹ , 1642 mAh g ⁻¹	0.2A g ⁻¹ , 100 cycles, 720 mAh g ⁻¹	Electrochim. Acta 2017 ⁶
1T-MoS ₂ nanoparticles, Super P	Hydrothermal method/DI	Coating separator	0.2C, 983 mAh g ⁻¹	0.2C, 150 cycles, 525 mAh g ⁻¹	Appl. Mater. Interfaces 2018 ⁷
1T-MoS₂, CFC	Hydrothermal method/DI	Self-supporting interlayer	0.2C, 1170 mAh g⁻¹	0.5C, 400 cycles, 497 mAh g⁻¹, CE=100%	This work

References

1. H. Zhao, H. Wu, J. Wu, J. Li, Y. Wang, Y. Zhang and H. Liu, Preparation of MoS₂/WS₂ nanosheets by liquid phase exfoliation with assistance of epigallocatechin gallate and study as an additive for high-performance lithium-sulfur batteries, *J Colloid Interface Sci*, 2019, **552**, 554-562.
2. Z.-L. Xu, N. Onofrio and J. Wang, Boosting the anchoring and catalytic capability of MoS₂ for high-loading lithium sulfur batteries, *Journal of Materials Chemistry A*, 2020, **8**, 17646-17656.
3. Y. C. Jeong, J. H. Kim, S. H. Kwon, J. Y. Oh, J. Park, Y. Jung, S. G. Lee, S. J. Yang and C. R. Park, Rational design of exfoliated 1T MoS₂@CNT-based bifunctional separators for lithium sulfur batteries, *Journal of Materials Chemistry A*, 2017, **5**, 23909-23918.
4. J. Li, Y. Jiang, F. Qin, J. Fang, K. Zhang and Y. Lai, Magnetron-sputtering MoS₂ on carbon paper and its application as interlayer for high-performance lithium sulfur batteries, *Journal of Electroanalytical Chemistry*, 2018, **823**, 537-544.
5. S. Liu, Z. Zhou and D. Liu, MoS₂ coated separator as an efficient barrier for inhibiting shuttle effect of polysulfide, *Ceramics International*, 2019, **45**, 14415-14419.
6. P. Guo, D. Liu, Z. Liu, X. Shang, Q. Liu and D. He, Dual functional MoS₂/graphene interlayer as an efficient polysulfide barrier for advanced lithium-sulfur batteries, *Electrochimica Acta*, 2017, **256**, 28-36.
7. P. Han, S. H. Chung and A. Manthiram, Thin-Layered Molybdenum Disulfide Nanoparticles as an Effective Polysulfide Mediator in Lithium-Sulfur Batteries, *ACS Appl Mater Interfaces*, 2018, **10**, 23122-23130.