

Supplementary Materials

MoO₃@MoS₂ Core-Shell Structured Hybrid Anode Materials for Lithium-Ion Batteries

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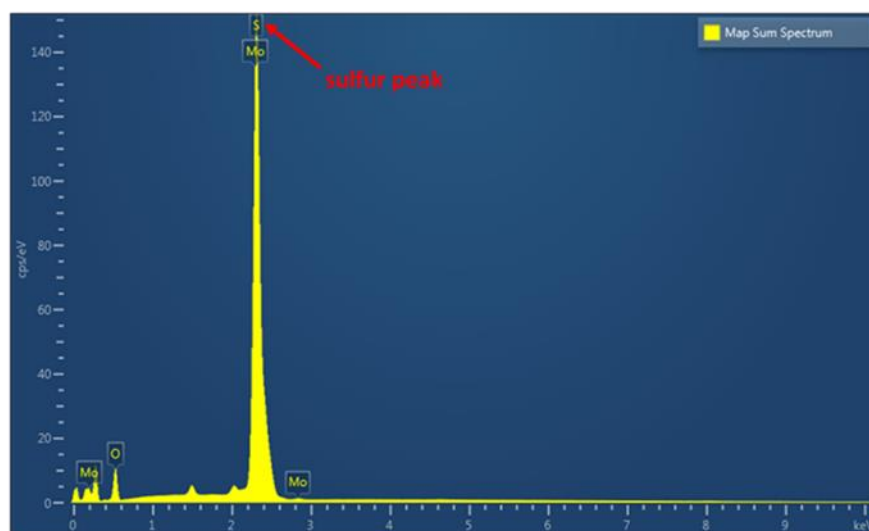


Figure S1. EDX spectrum of $\text{MoO}_3@\text{MoS}_2$.

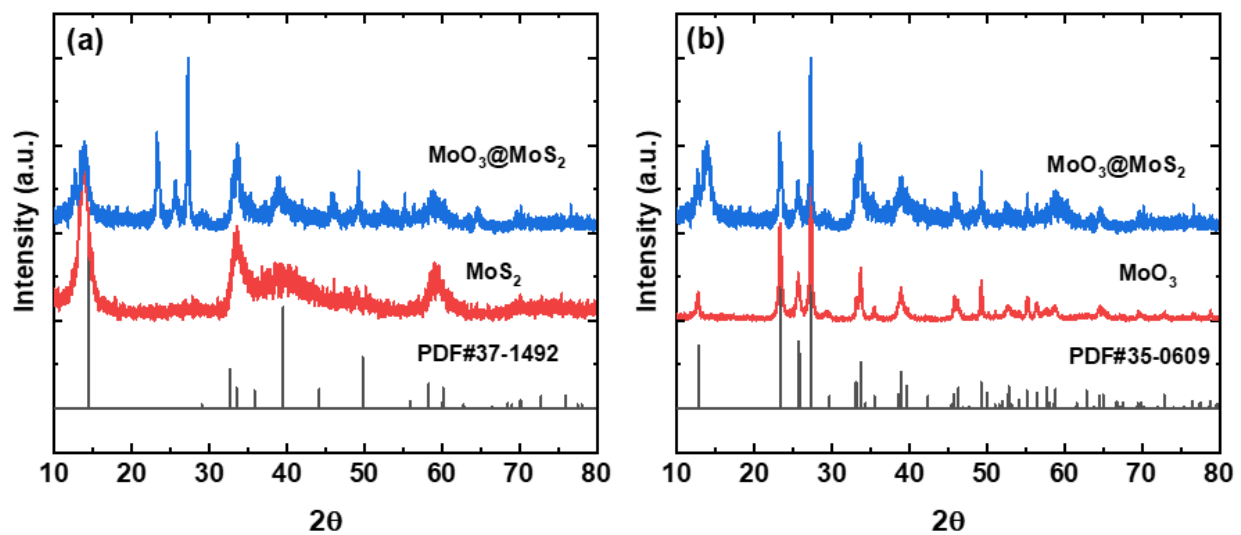


Figure S2. XRD of (a) MoS_2 and (b) MoO_3 , including $\text{MoO}_3@\text{MoS}_2$, compared with their corresponding standard (PDF) data.

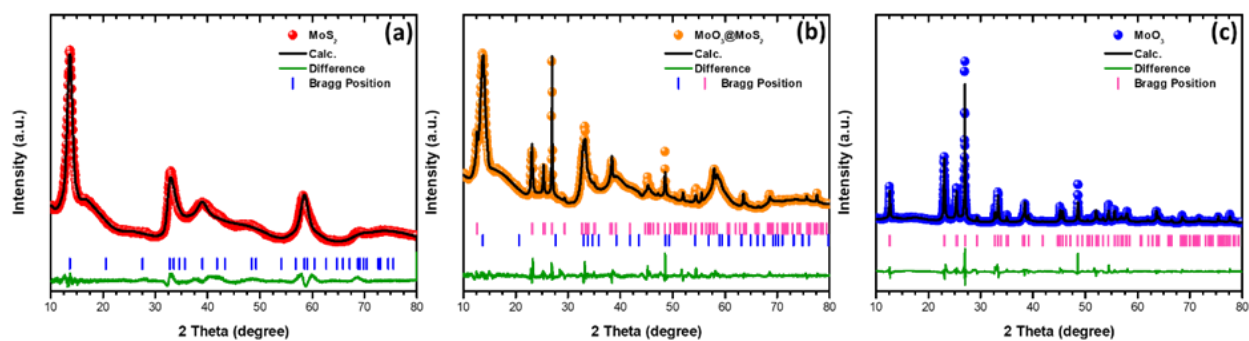


Figure S3. Profile matching of HRPD data of (a) MoS_2 , (b) $\text{MoO}_3@/\text{MoS}_2$, and (c) MoO_3 .

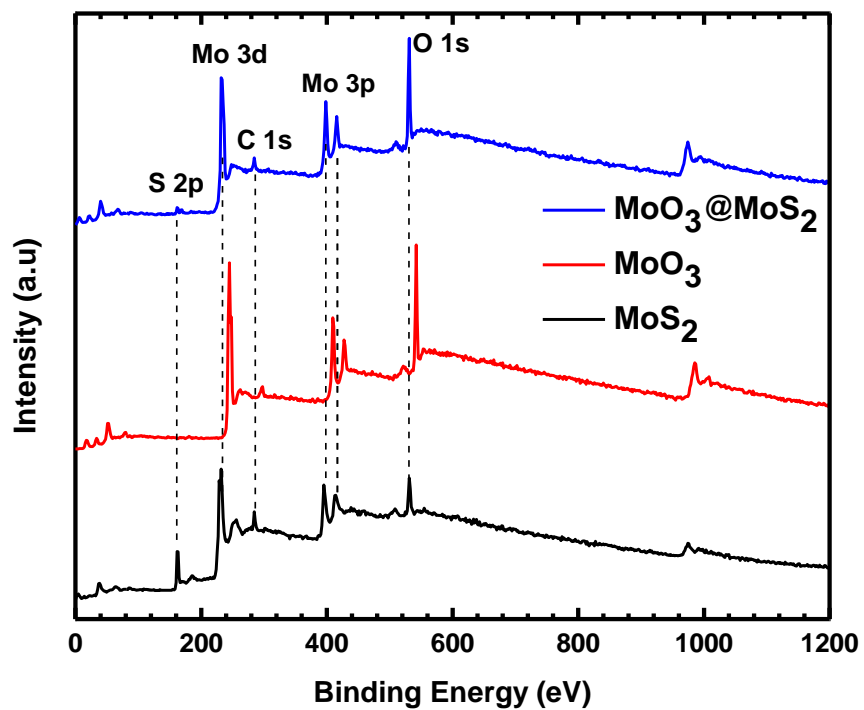


Figure S4. XPS survey spectrum of MoS_2 , MoO_3 , and $\text{MoO}_3@/\text{MoS}_2$.

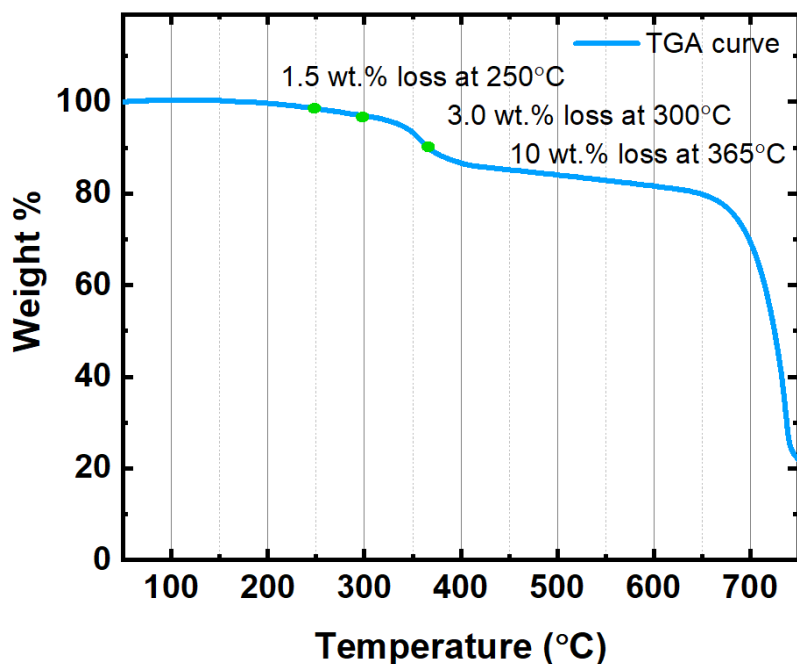


Figure S5. Thermogravimetric analysis (TGA) curve of as-synthesized MoS₂ in air.

Calculation of the ratio of MO₃ to MS₂ in the MoO₃@MoS₂.

MoS₂ (Mw: 160.07 g/mol) and MoO₃ (Mw: 143.94 g/mol)

If MoS₂ is fully decomposed to MoO₃,

$$\text{MoO}_3/\text{MoS}_2 = 143.94 / 160.07 = 0.899 \Rightarrow \text{then } 10 \text{ wt}\% \text{ decrease}$$

From the TGA data, we observed 1.5 wt% loss after the oxidation process above 250 °C. Therefore, we can determine that MoS₂:MoO₃ ratio is approximately 8.5:1.5 in **MoO₃@MoS₂** hybrid based on the TGA data.

The **MoO₃@MoS₂** hybrid anode theoretical capacity (1 C= 737 mAh g⁻¹) calculated by the rule of mixtures of the two active materials:

$$(C_{\text{MoO}_3@\text{MoS}_2} = C_{\text{MoS}_2} \times 0.85 + C_{\text{MoO}_3} \times 0.15 = 670 \text{ mAh g}^{-1} \times 0.85 + 1117 \text{ mAh g}^{-1} \times 0.15).$$

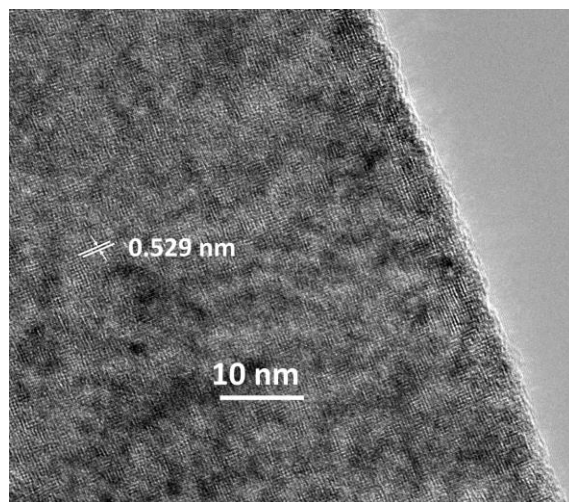


Figure S6: HR-TEM image of the MoO₃@MoS₂ sample.

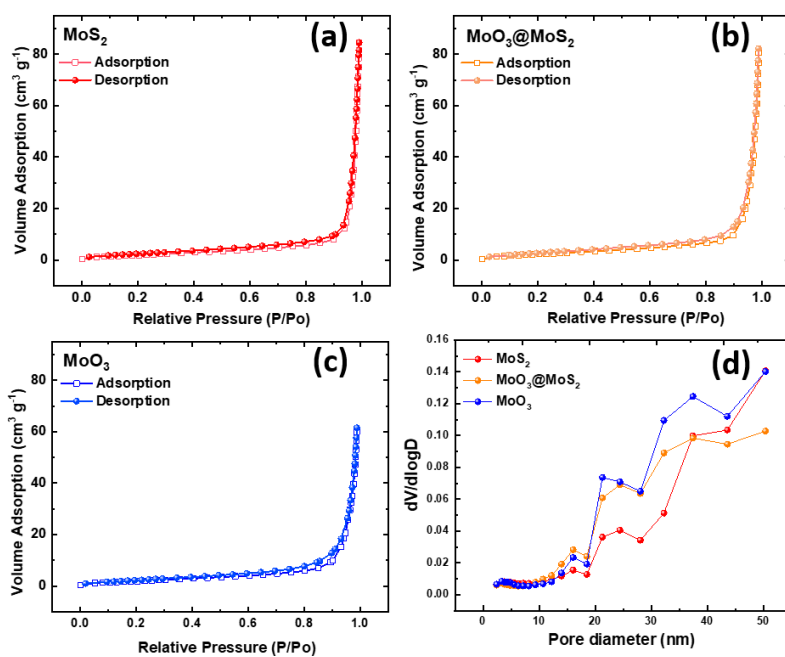


Figure S7. (a-c) BET and (d) corresponding BJH profile of MoS₂, MoO₃, and MoO₃@MoS₂.

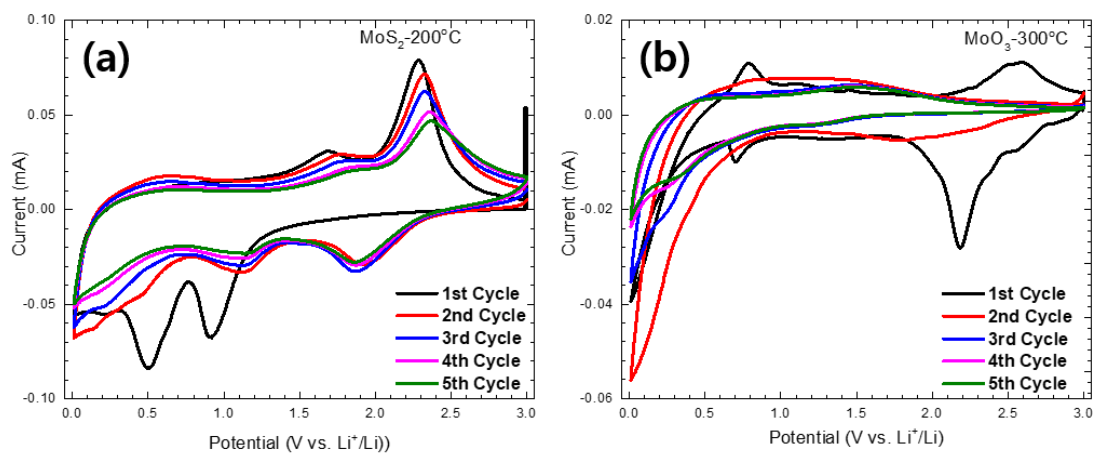


Figure S8. CV curves of (a) MoS₂ and (b) MoO₃ anodes.

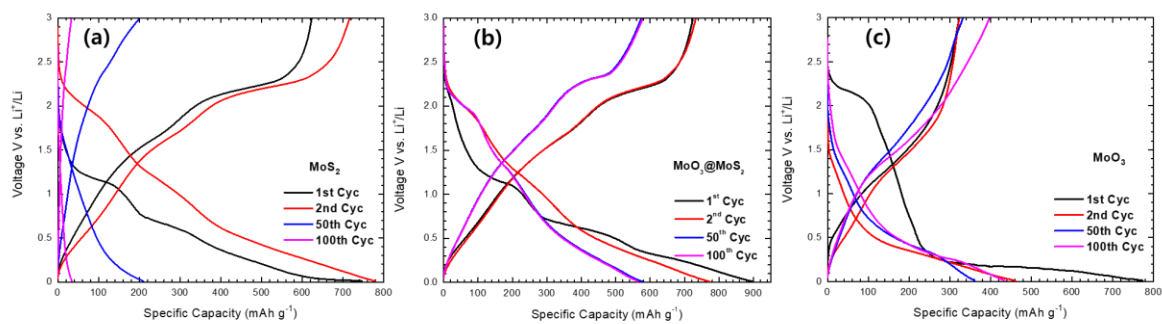


Figure S9. GCD curves of the (a) MoS₂, (b) MoO₃@MoS₂ and (c) MoO₃.

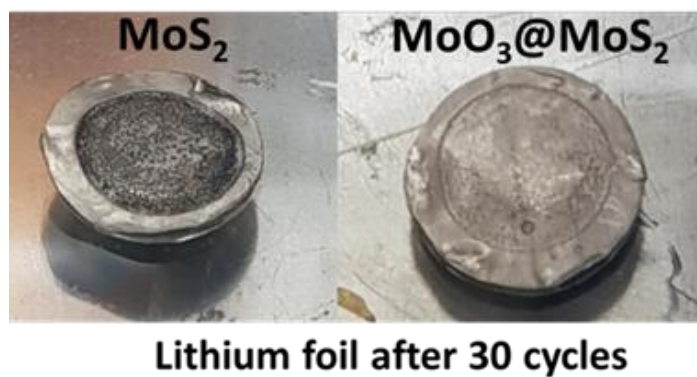


Figure S10. Photos of Li counter electrodes for the MoS_2 and $\text{MoO}_3@\text{MoS}_2$ electrodes half-cells.

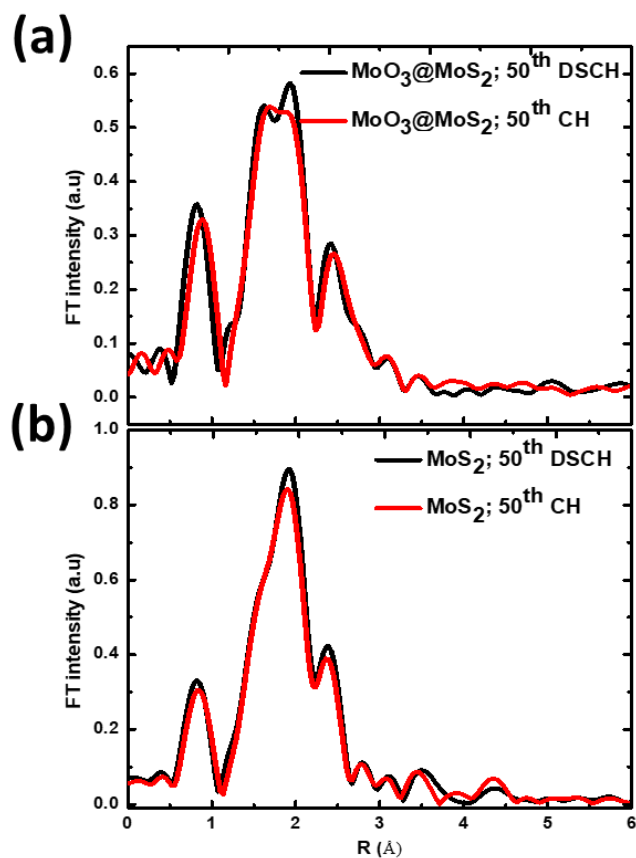


Figure S11. Ex-situ Mo k-edge FT-EXAFS spectra of MoS_2 and $\text{MoO}_3@\text{MoS}_2$ after 50 cycles.

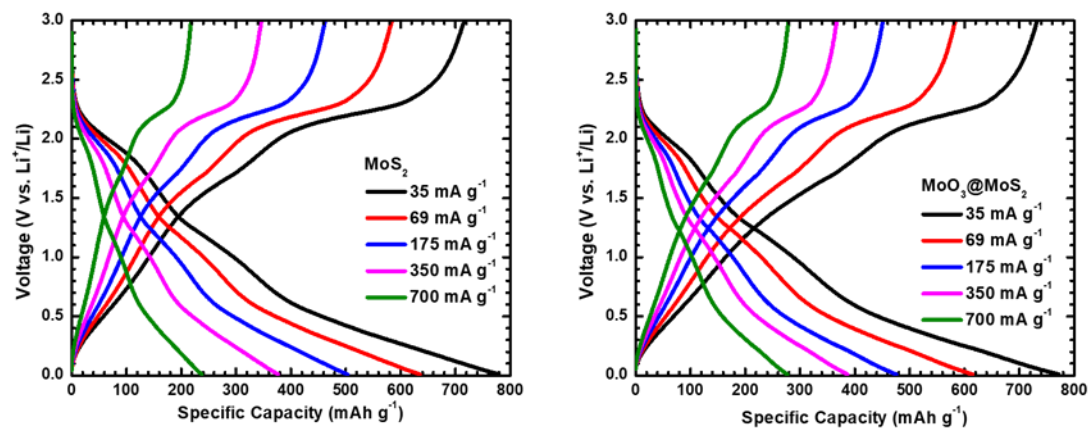


Figure S12. The galvanostatic voltage profiles (rate performance) of MoS_2 and $\text{MoO}_3@\text{MoS}_2$ anodes at different current densities in LIBs.

Table S1. Unit cell parameters of MoS₂, MoO₃@MoS₂, and MoO₃.

	MoS ₂			MoO ₃			
	(a,b) Å	(c) Å	(v) Å ³	(a) Å	(b) Å	(c) Å	(v) Å ³
MoS ₂	3.1132	12.7912	107.3655				
MoO ₃ @MoS ₂	3.0938	12.7677	105.8369	3.9518	13.8893	3.7001	203.0908
MoO ₃				3.9615	13.8737	3.6981	203.254

Table S2. Result of BET analysis of MoS₂, MoO₃@MoS₂, and MoO₃.

Sample	BET (m ² g ⁻¹)	Pore volume (cm ³ g ⁻¹)	Mean pore diameter (nm)
MoS ₂	8.71	0.1011	46.423
MoO ₃ @MoS ₂	8.42	0.129	61.61
MoO ₃	9.85	0.1317	53.455

Table S3. Fitted solution resistance (R_s) and charge transfer resistance (R_{ct}) values of MoS₂, MoO₃@MoS₂, and MoO₃ after 1st cycle.

Sample	R _s (Ω)	R _{ct} (Ω)
MoS ₂	82.26	473.24
MoO ₃ @MoS ₂	2.392	284.308
MoO ₃	6.656	518.44

Table S4. Fitted solution resistance (R_s) and charge transfer resistance (R_{ct}) values of MoS₂, MoO₃@MoS₂, and MoO₃ after 30th cycle.

Sample	R _s (Ω)	R _{ct} (Ω)
MoS ₂	75.77	728.33
MoO ₃ @MoS ₂	6.261	304.539
MoO ₃	2.476	700

Table S5. Comparative table depicting electrochemical performance of selected TMO/TMS and/or carbon hybrids.

Materials	Current density (mA g ⁻¹)	Cycle number	Reversible capacity (mAh g ⁻¹)	References
SnS ₂ /SnO ₂	100	80	520	[1]
MoO ₃ /SnS ₂	100	100	504	[2]
TiO ₂ @MoS ₂	100	100	544	[3]
VS ₂ @CNT	200	100	850	[4]
MoS ₂ /MoO ₃ /N-doped carbon	1000	350	887.5	[5]
MoSe ₂ @porous hollow carbon spheres (PHCS)	1000	100	681	[6]
Si@Li ₄ Ti ₅ O ₁₂	500	150	883	[7]
MoO₃@MoS₂	50	100	564	This work

References

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