Supporting Information

CMK-5-encapsulated MoSe₂ Composite for Rechargeable Lithium-ion Batteries with Improved Electrochemical Performance

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Preparation of CMK-5

CMK-5 was prepared by using SBA-15 as hard template. Typically, 2 g of P123 (EO₂₀PO₇₀EO₂₀, Sigma-Aldrich) was added into 130 mL HCl solution (0.8 M) at 35 °C and was vigorously stirred till P123 was dissolved. Subsequently, 4.2 g of tetraethyl orthosilicate (TEOS) was added to the above solution rapidly. After being stirred for 5 min, the mixture was placed at a static condition at 35 °C for 24 h and at 130 °C for another 24 h. The SBA-15 template was obtained after the white precipitate was filtered, dried without washing, and calcined at 550 °C for 6 h. Then the SBA-15 powder was impregnated with aqueous solution of AlCl₃ (with a molar ratio of Si/Al = 20). After the solvent water was completely evaporated at room temperature, the samples were dried at 70 °C and calcined in air at 550 °C for 6 h. The aluminosilicate SBA-15 (Al-SBA-15) was incorporated with furfuryl alcohol (FA) at a mass ratio of 1:1.3 by incipient wetness infiltration. The FA/Al-SBA-15 mixture was then heated at 80 °C for 4 h and 150 °C for 8 h. Subsequently, the FA/Al-SBA-15 mixture was heated at 80 °C in vacuum condition for another 1 h. Then the dark brown powder was carbonized at 900 °C in Ar flow for 6 h. The CMK-5 was obtained after the removal of SBA-15 template by 5% HF acid at room temperature.





Fig. S1 Schematic illustration for the synthetic procedure of the MoSe₂/CMK-5 composite.



Fig. S2 SEM images of (a) bulk MoSe₂ and (b) mechanically mixed MoSe₂&CMK-5.



Fig. S3 Magnified TEM image of the CMK-5.



Fig. S4 Low-angle XRD patterns of the as-obtained (a) SBA-15 template (after calcination in air at 550 °C for 6 h) and (b) CMK-5.



Fig. S5 (a, b) TEM images and (c) HRTEM image of bulk MoSe₂.



Fig. S6 Charge/discharge profiles of the MoSe₂/CMK-5 composite at the current density of 1000 mA g⁻¹ within a voltage window of 0.01-3

V.



Fig. S7 Comparison of cycling performance of MoSe₂/CMK-5 composite, pure CMK-5 bulk MoSe₂ and MoSe₂&CMK-5 at a current density of

1000 mA g⁻¹.

Table S1. Comparison of the electrochemical properties of MoSe₂-based anode materials for LIBs.

Electrode material	High rate capacity/mA h g ⁻¹ (Current density/mA g ⁻¹)	Cycling performance		
		Current density/mA g ⁻¹	Capacity/mA h g ⁻¹ (Cycle number)	– Ref.
MoSe ₂ /CMK-5 composite	542 (2000)	100 1000 2000	788 (100) 567 (100) 451 (1000)	This work
MoSe ₂ /rGO	436 (2000)	100 1000 2000	714 (100) 637 (1000) 425 (1000)	1
3D MoSe ₂ /rGO foam	330 (844, 2C)	42.2, 0.1C 211, 0.5C	650 (50) 470 (600)	2
MoO2@MoSe2	485 (2000)	2000	520 (400)	3
MoSe ₂ /graphene hybrids	667 (1000)	100	1102 (100)	4
Sheet-like MoSe ₂ /C composites	450 (2000)	100	577 (50)	5
Mesoporous MoSe ₂	372 (844, 2C)	21.1, 0.05C	630 (35)	6
MoSe ₂ @ PHCS	640 (3000)	1000	792 (100)	7
Coaxial-cable MoSe ₂ /C composites	524 (3000)	500	632 (100)	8
MoSe ₂ /rGO composite	750 (1000)	500	917 (100)	9

For most of the reported MoSe₂-based anode materials, the cycle numbers are 100 or less than 100, even though some of them exhibited high capacities over 790 mA h g⁻¹. ^{4, 7, 9} However, those with cycle numbers up to 500 are still rare. ^{1, 2} MoSe₂/rGO hybrids reported by Luo et al. ¹ demonstrated a good cycling stability up to 1000 cycles, but the high rate capability was inferior. The 3D MoSe₂/rGO foam showed a good capacity retention for 600 cycles, ² but the reversible capacity was dissatisfactory even cycled at a very low rate. Therefore, the MoSe₂/CMK-5 in this work demonstrates outstanding electrochemical properties considering the current rate and the cycling life.

References

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