Supplementary Material

Synergistic design of semi-hollow core-shell structure and metal organic framework derived Co/Zn selenide coated with MXene for high-performance lithium-sulfur batteries

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Supplementary materials include: The preparation process of 45@ZnSe-CoSe/P/S composite; SEM images of ZIF-8 and ZIF-8@ZIF-67; XRD patterns of ZIF-8, ZIF-8@ZIF-67 and different hollow degree of ZIFs; N2 adsorption-desorption isotherms of four HZIFs; XRD patterns of electrode materials after sulfur loading; XPS spectra of 45@ZnSe-CoSe/M; TGA curves of 45@ZnSe-CoSe/P/S and 45@ZnSe-CoSe/M/S; The initial discharge/charge curves of 15@ZnSe-CoSe/S, 30@ZnSe-CoSe/S, 60@ZnSe-CoSe/S and 45@ZnSe-CoSe/P/S at various current rates; CV curves of 15@ZnSe-CoSe/S, 30@ZnSe-CoSe/S, 60@ZnSe-CoSe/S and 45@ZnSe-CoSe/P/S at scanning rates ranging from 0.1 to 0.4 mV s^{-1}; The scanning rate-dependent peak currents for the calculation of Li+ diffusion coefficients.

1. Synthesis of 45@HZIF/PDA

45@HZIF (200 mg) was uniformly dispersed in 200 mL Tris solution (pH = 8.5) and ultrasonically oscillated for 10 min. Subsequently, 200 mg of dopamine hydrochloride was introduced into the above mixture and continuously stirred at room

temperature for 3 hours. The sediment was collected by centrifugation, washed with deionized water and anhydrous ethanol, and finally dried for 12 hours at 60 °C in air.

2. Synthesis of 45@ZnSe-CoSe/P

1 g Se powder in a porcelain boat was placed in upstream and 0.5 g 45@HZIF/PDA was placed in downstream of a tube furnace. Then, the materials in the porcelain boats were reacted at 800 °C for 3 hours with a heating rate of 2 °C min^{-1} under an N_2 atmosphere. Finally, the product of 45@ZnSe-CoSe/P hollow polyhedron was obtained.

3. Synthesis of 45@ZnSe-CoSe/P/S composite

Typically, the as-prepared 45@ZnSe-CoSe/P and sublimed sulfur were thoroughly ground for about 30 min in a mortar at a weight ratio of 1:3. Then, the hybrid was put into a glass bottle and heated at 155 ℃ for 12 hours in vacuum to obtain 45@ZnSe-CoSe/P/S.

4. Adsorption of lithium polysulfides

Lithium sulfide (Li_2S) and sulfur powders with a stoichiometric molar ratio of 1:5 were added into a certain amount of 1,3-dioxolane (DOL) and 1,2-dimethoxyethane (DME) [1:1 in vol] solvents. Then, the mixture was stirred at 80 °C until the solid was fully dissolved. Typically, 20 mg of 45@ZnSe-CoSe/M or 45@ZnSe-CoSe was placed in 5 mL of Li_2S_6 (2 mmol/L), and the mixture was static adsorption for 5 hours.

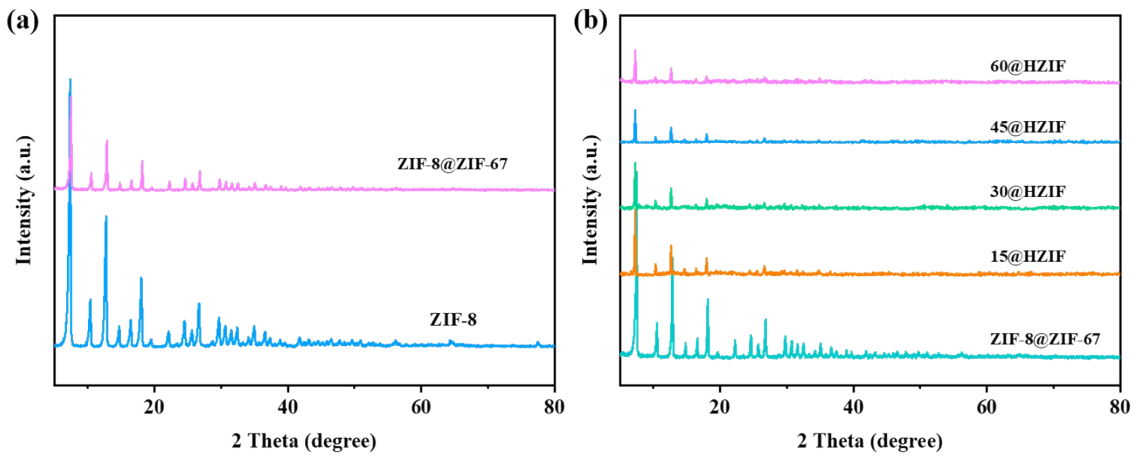

Fig. S1 (a) XRD patterns of ZIF-8 and ZIF-8@ZIF-67. (b) XRD patterns of 15@HZIF, 30@HZIF, 45@HZIF and 60@HZIF.

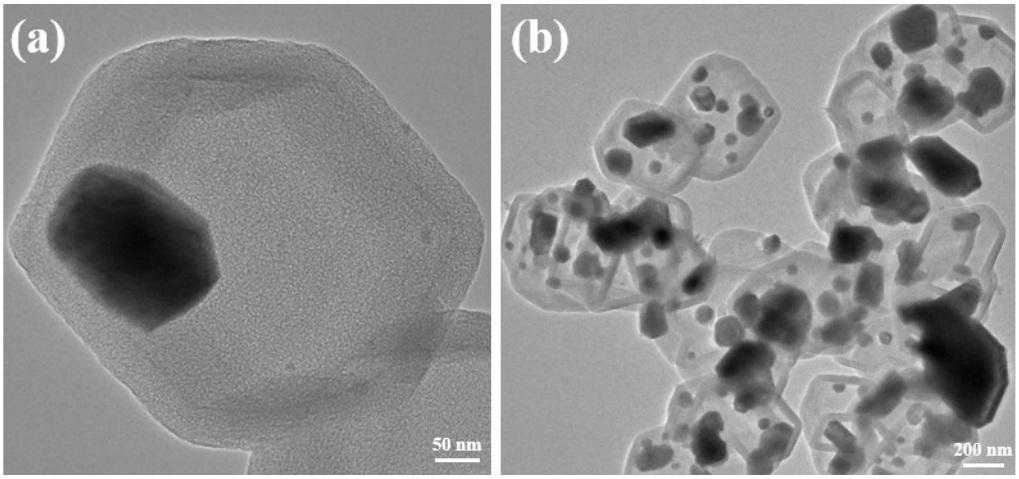

Fig. S2 TEM images of 45@ZnSe-CoSe.

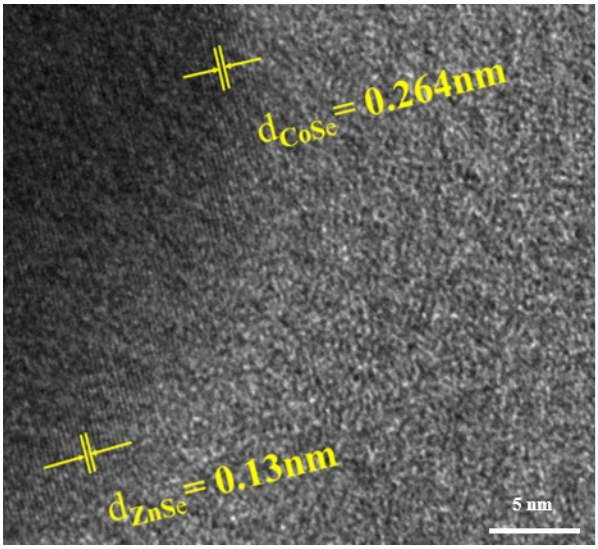

Fig. S3 HRTEM images of 45@ZnSe-CoSe.

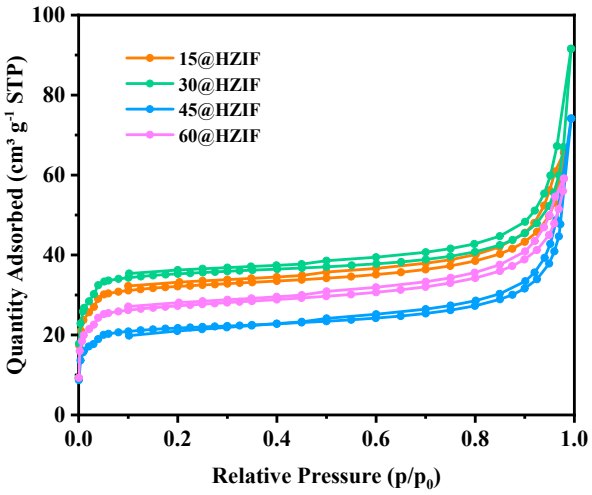

Fig. S4 N_2 adsorption-desorption isotherms :15@HZIF, 30@HZIF, 45@HZIF and 60@HZIF.

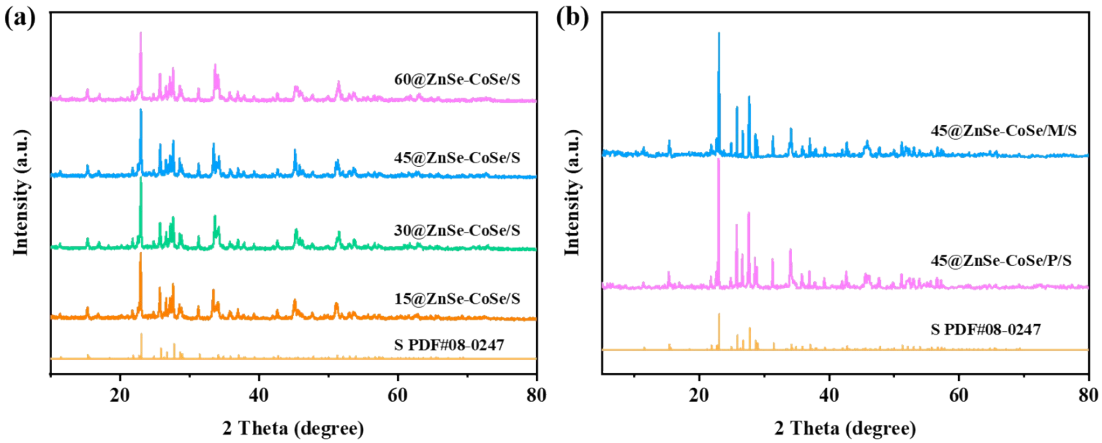

Fig. S5 (a) XRD patterns of 15@ZnSe-CoSe/S, 30@ZnSe-CoSe/S, 45@ZnSe-CoSe/S and 60@ZnSe-CoSe/S. (b) XRD patterns of 45@ZnSe-CoSe/P/S and 45@ZnSe-CoSe/M/S.

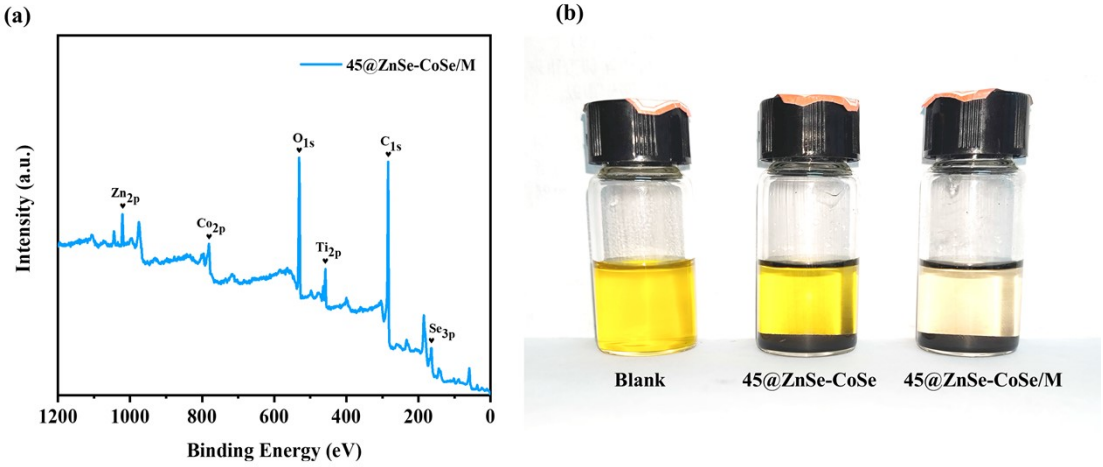

Fig. S6 (a) XPS spectra of 45@ZnSe-CoSe/M, (b) The static lithium polysulfide adsorption tests

for 45@ZnSe-CoSe and 45@ZnSe-CoSe/M.

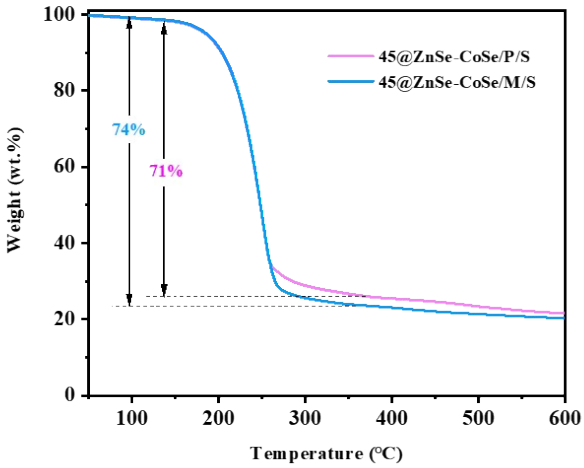

Fig. S7 TGA curves of 45@ZnSe-CoSe/P/S and 45@ZnSe-CoSe/M/S in the temperature range of 50-500 °C.

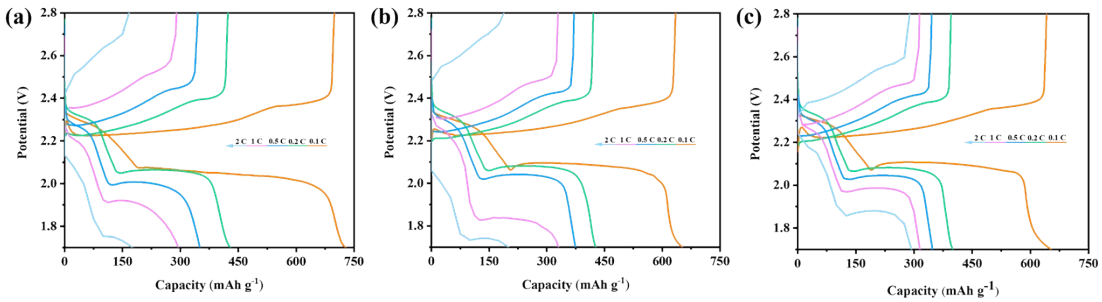

Fig. S8 The initial discharge/charge curves of 15@ZnSe-CoSe/S, 30@ZnSe-CoSe/S and 60@ZnSe-CoSe/S at various current rates.

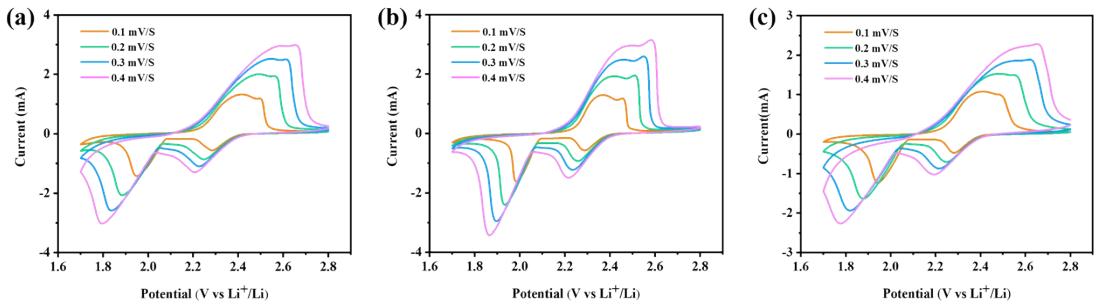

Fig. S9 CV curves of 15@ZnSe-CoSe/S, 30@ZnSe-CoSe/S and 60@ZnSe-CoSe/S at scanning rates ranging from 0.1 to 0.4 mV s^{-1}.

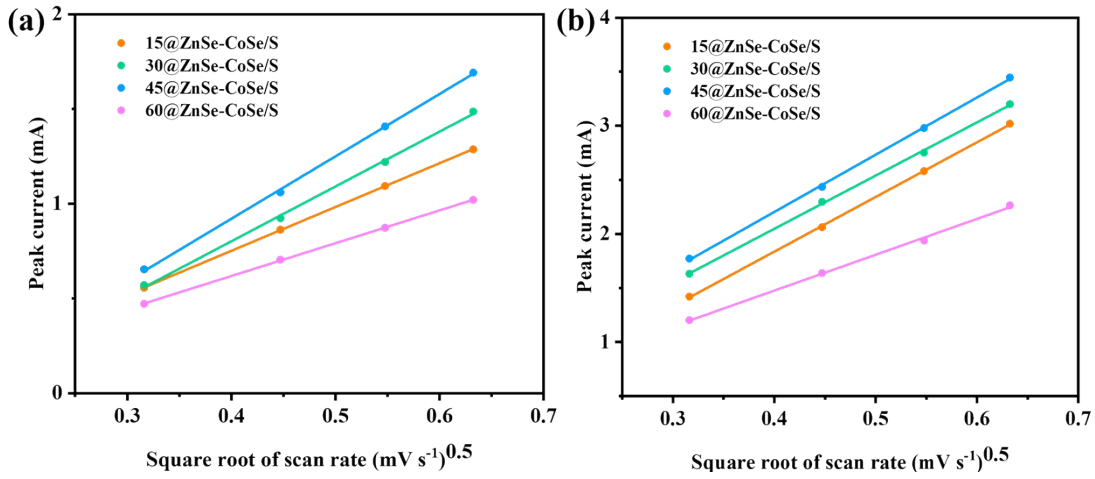

Fig. S10 The scanning rate-dependent peak currents at C1 and C2 positions for the calculation of Li^+ diffusion coefficients.

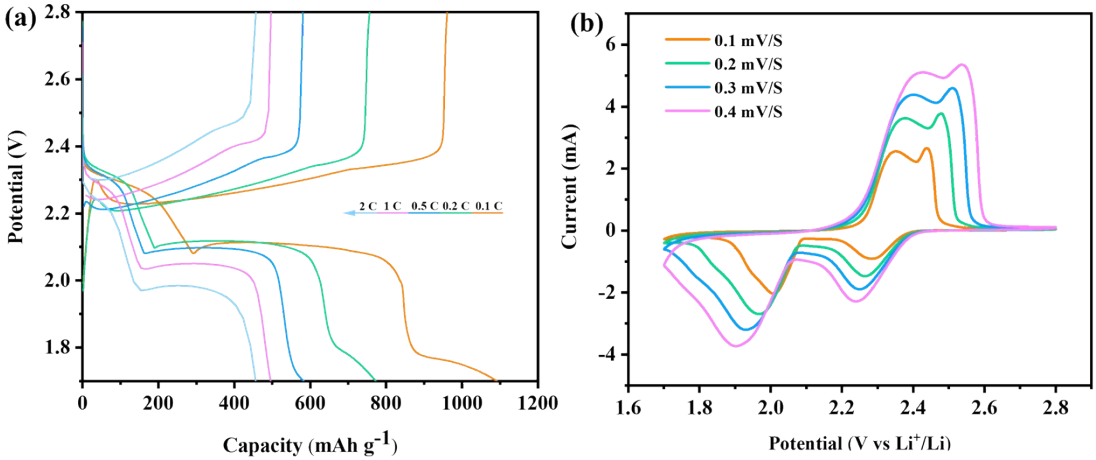

Fig. S11 (a) The initial discharge/charge curves of 45@ZnSe-CoSe/P/S at various current rates. (b) CV curves of 45@ZnSe-CoSe/P/S at scanning rates ranging from 0.1 to 0.4 mV s^{-1}.

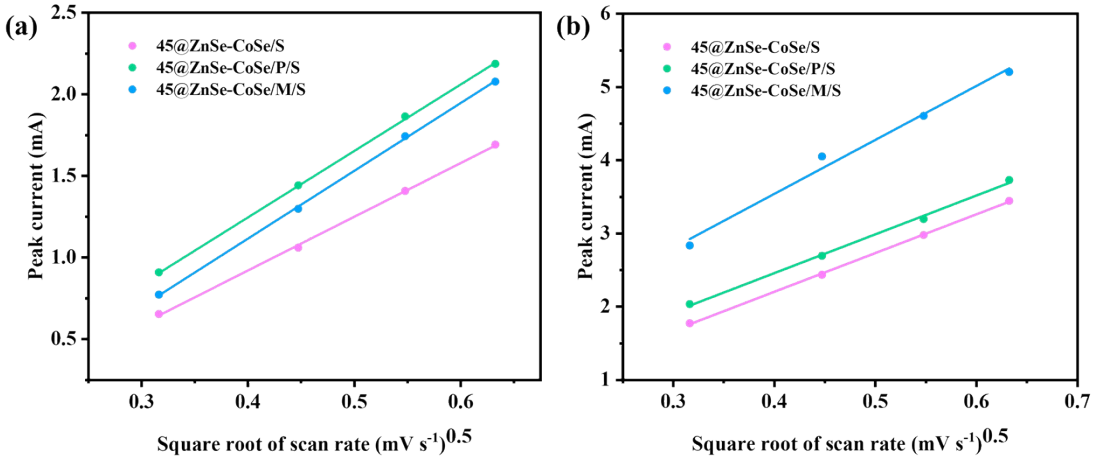

Fig. S12 The scanning rate-dependent peak currents at C1 and C2 positions for the calculation of Li^+ diffusion coefficients.

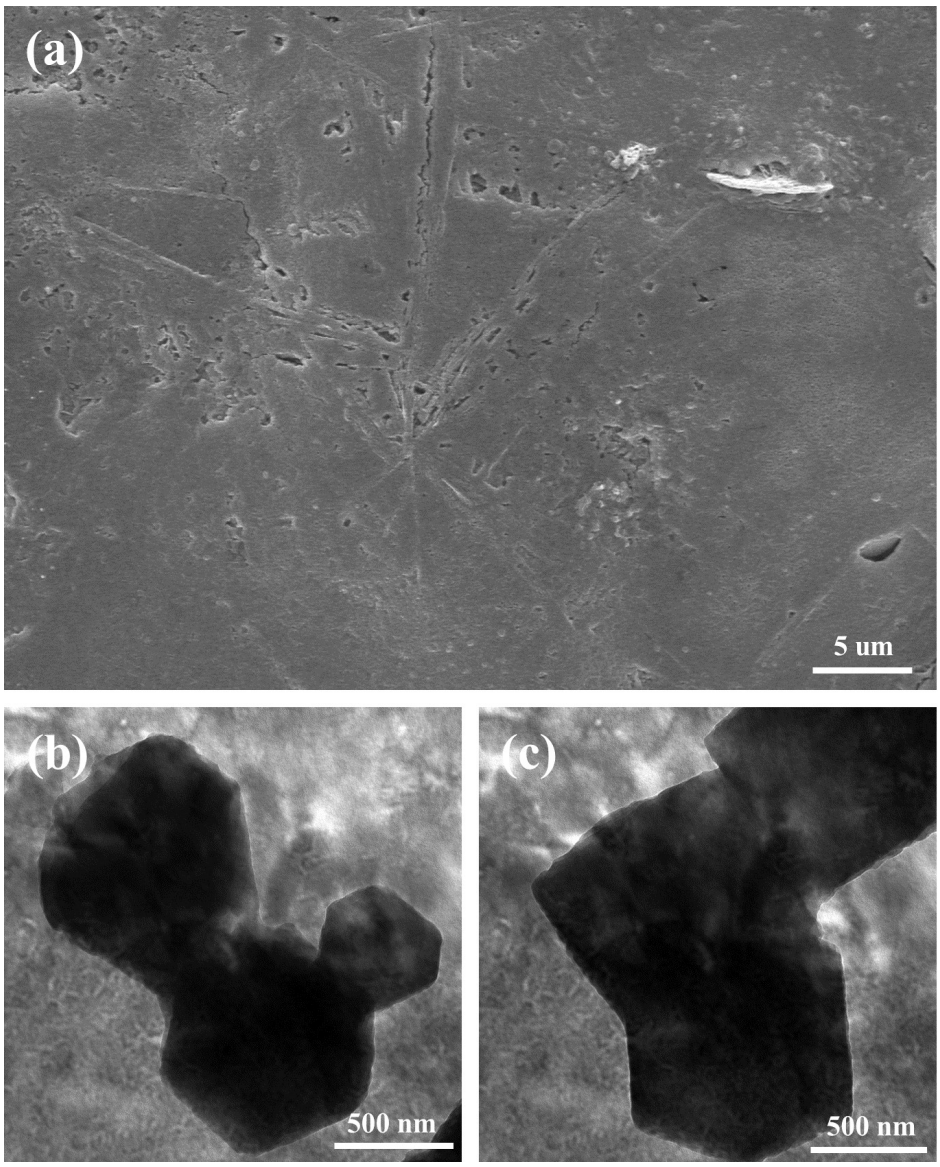

Fig. S13 (a) The SEM and (b, c) TEM images of 45@ZnSe-CoSe/M/S electrode after 80 cycles.