



Supporting Information

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Enhanced Sulfur Transformation by Multifunctional FeS₂/FeS/S Composites for High-Volumetric Capacity Cathodes in Lithium–Sulfur Batteries

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Keywords: Lithium-sulfur batteries; FeS₂/FeS/S composites; Volumetric energy density; DFT calculations; Catalytic effect.

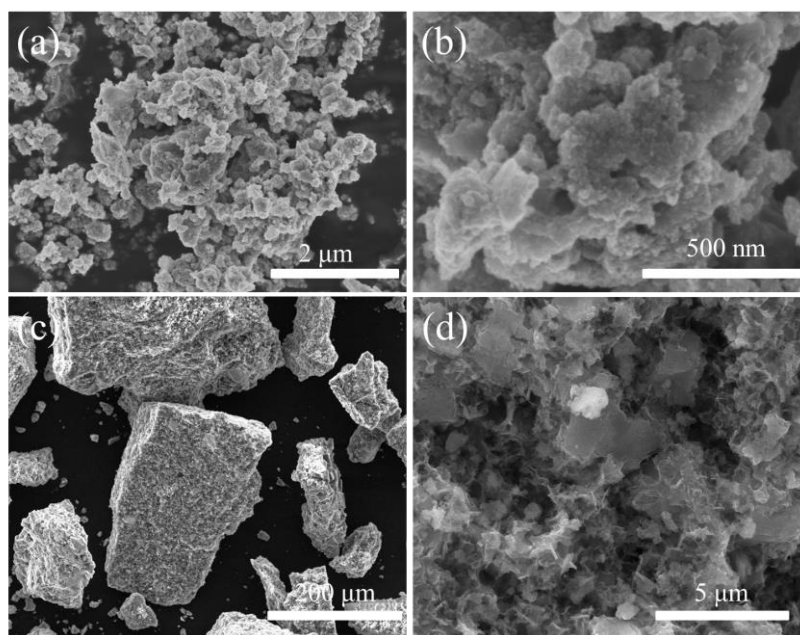


Figure S1. (a,b) SEM images of FeS₂/FeS/S composites after washing with trichloromethane (0.1g composite in 100 mL solvent); (c,d) SEM images of the ball-milled sample without washing.

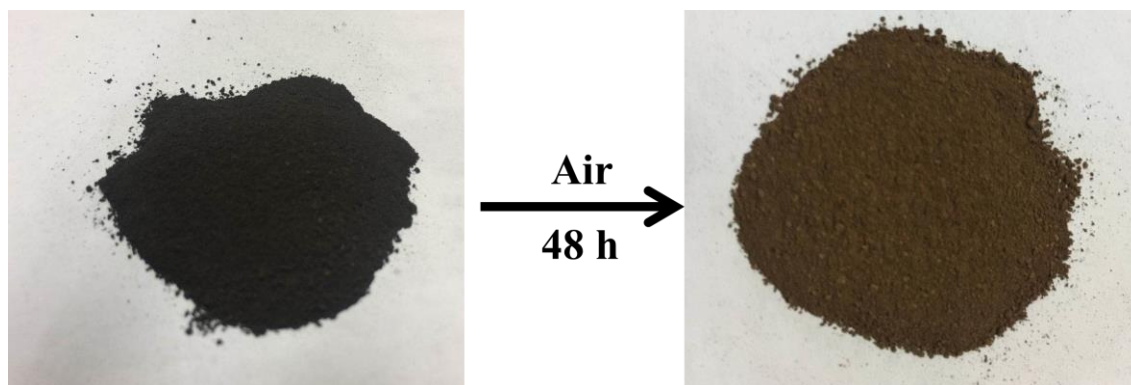


Figure S2. Colour comparisons of FeS₂/FeS/S composites before and after air exposure for 48 h.

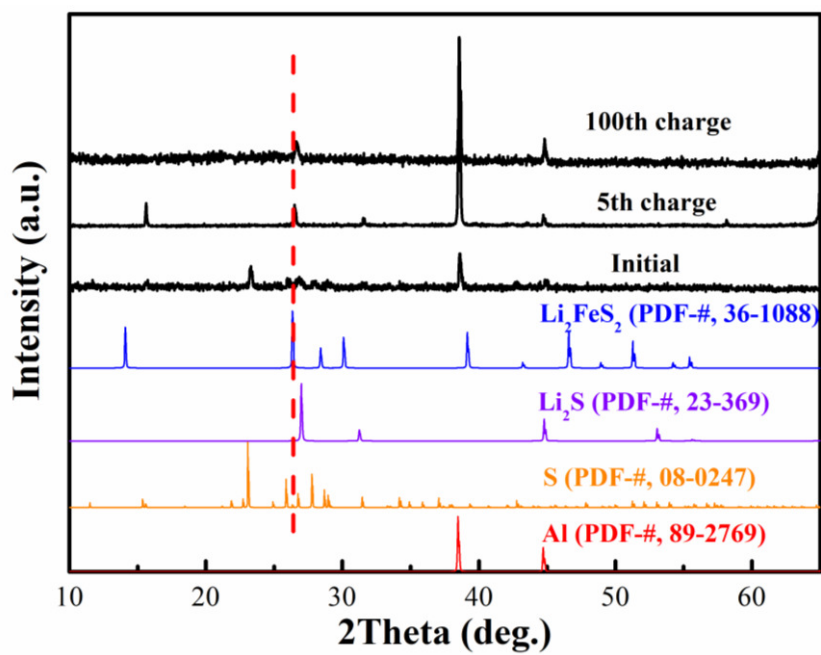


Figure S3. XRD spectra of FeS₂/FeS/S composites electrodes after various cycling times.

Table S1. Comparisons of the volumetric capacity of FeS₂/FeS/S composites and reported sulfur-based cathodes.

| Materials | Volumetric capacity (Ah·L ⁻¹) | Ref |
|-------------------------|---|--|
| FeS ₂ /FeS/S | 1491.7 (30cycle, 0.1C) 746.9 (200cycle, 1.0C) based on electrode | This work |
| rGO-VS ₂ /S | 1182.1 (100cycle, 0.1C) based on electrode | Advanced Energy Materials, 2017: 1702337 |
| Aligned CNT/S | 1116 (5cycle, 0.1C) based on electrode | Nano Energy, 2014, 4(2): 65-72 |
| MNCS/CNT-S | 1140 (200cycle, 1.68 mA·cm ⁻²) based on sulfur(56% in electrode) | Angewandte Chemie, 2015, 54(14): 4325-4329 |
| PSC-CNT-S | 800 (80cycle, 0.84mA·cm ⁻²) based on sulfur | Acs Applied Materials & Interfaces, 2013, 5(21): 11355-11362 |
| ρPAN-KB/S | 576 (100cycle, 0.5C) based on sulfur | Journal of Power Sources, 2016, 302: 70–78 |
| Nafion-coated FGSS | 870 (1cycle, 0.1C) based on electrode | Physical Chemistry Chemical Physics Pccp, 2011, 13(17): 7660-7665 |
| GGs | Below 450 (50cycle, 0.1C) based on electrode | Rsc Advances, 2015, 5(59): 47621-47627 |

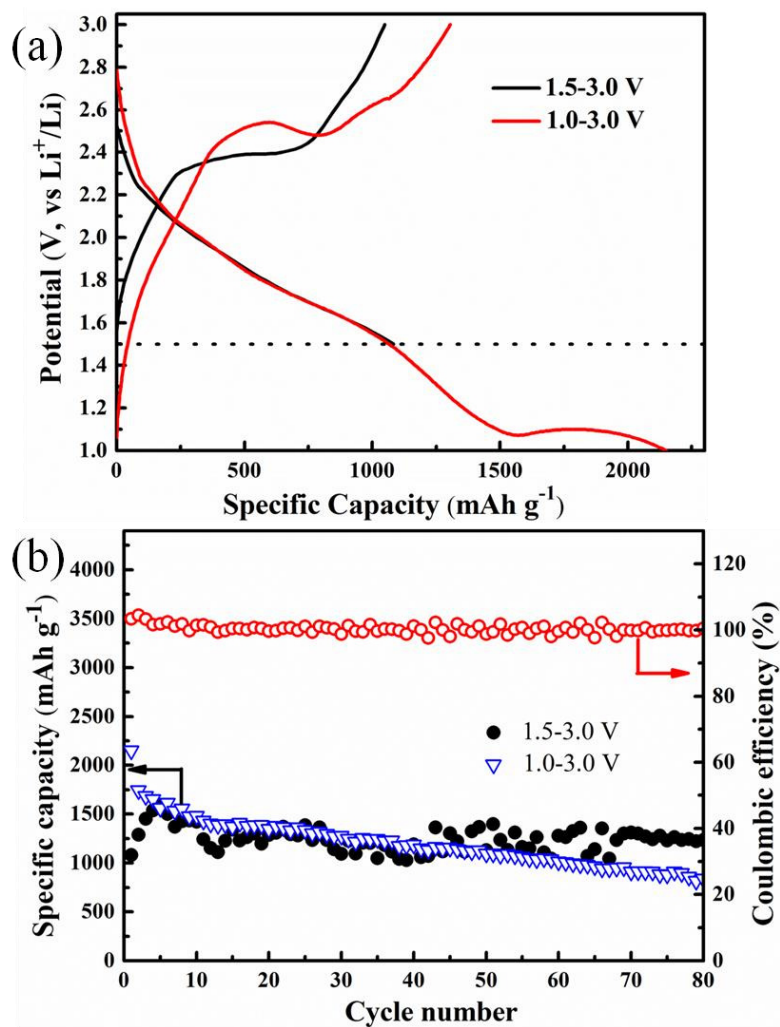


Figure S4. Discharge-charge curves (a) and cycle performance of FeS₂/FeS/S composites at a current density of 300 mA g⁻¹ at various cut-off potentials.

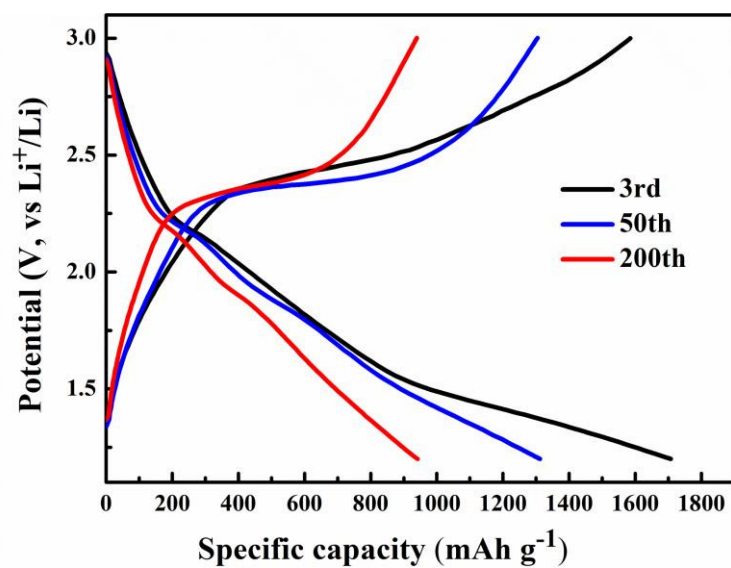


Figure S5. Discharge-charge curves of FeS₂/FeS/S composites at a current density of 1600 mA g⁻¹.

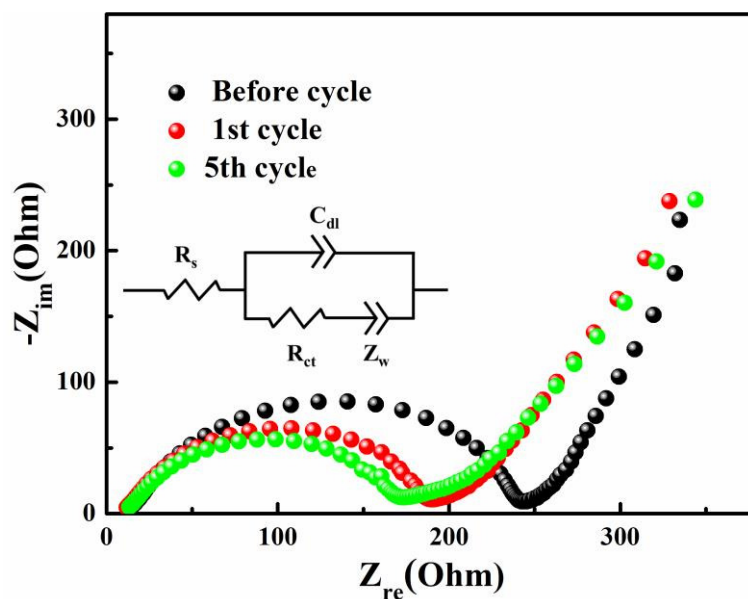


Figure S6. Electrochemical impedance spectroscopy of FeS₂/FeS/S composites.

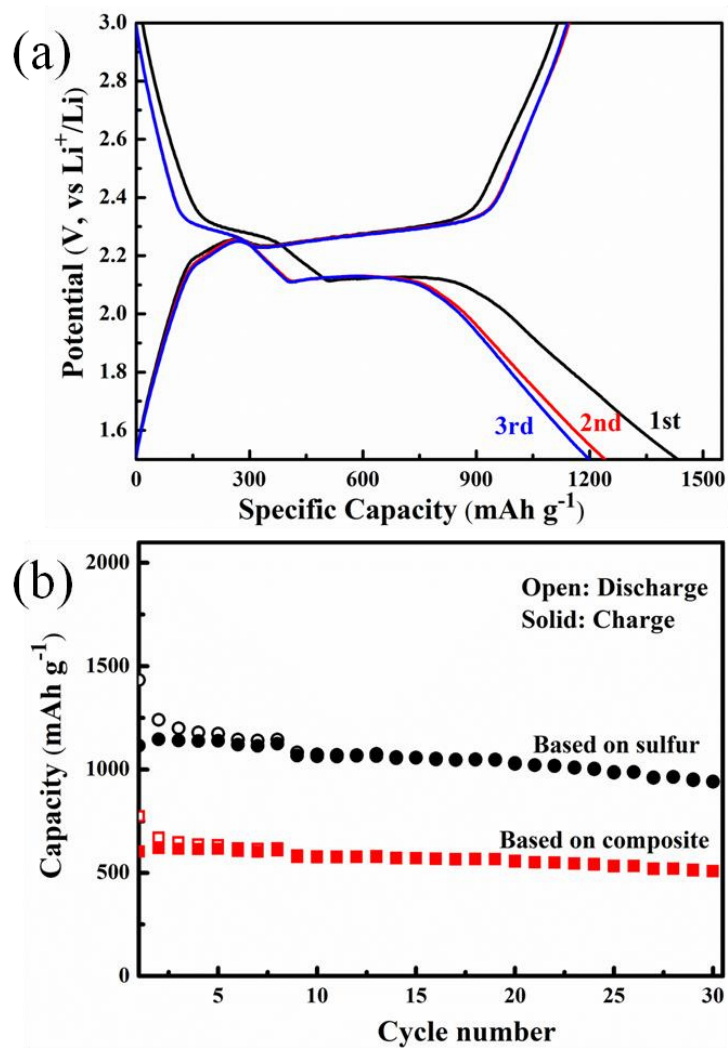


Figure S7. Discharge-charge curves (a) and cycle performance of conventional S/CNT composites at a current density of 160 mA g⁻¹.

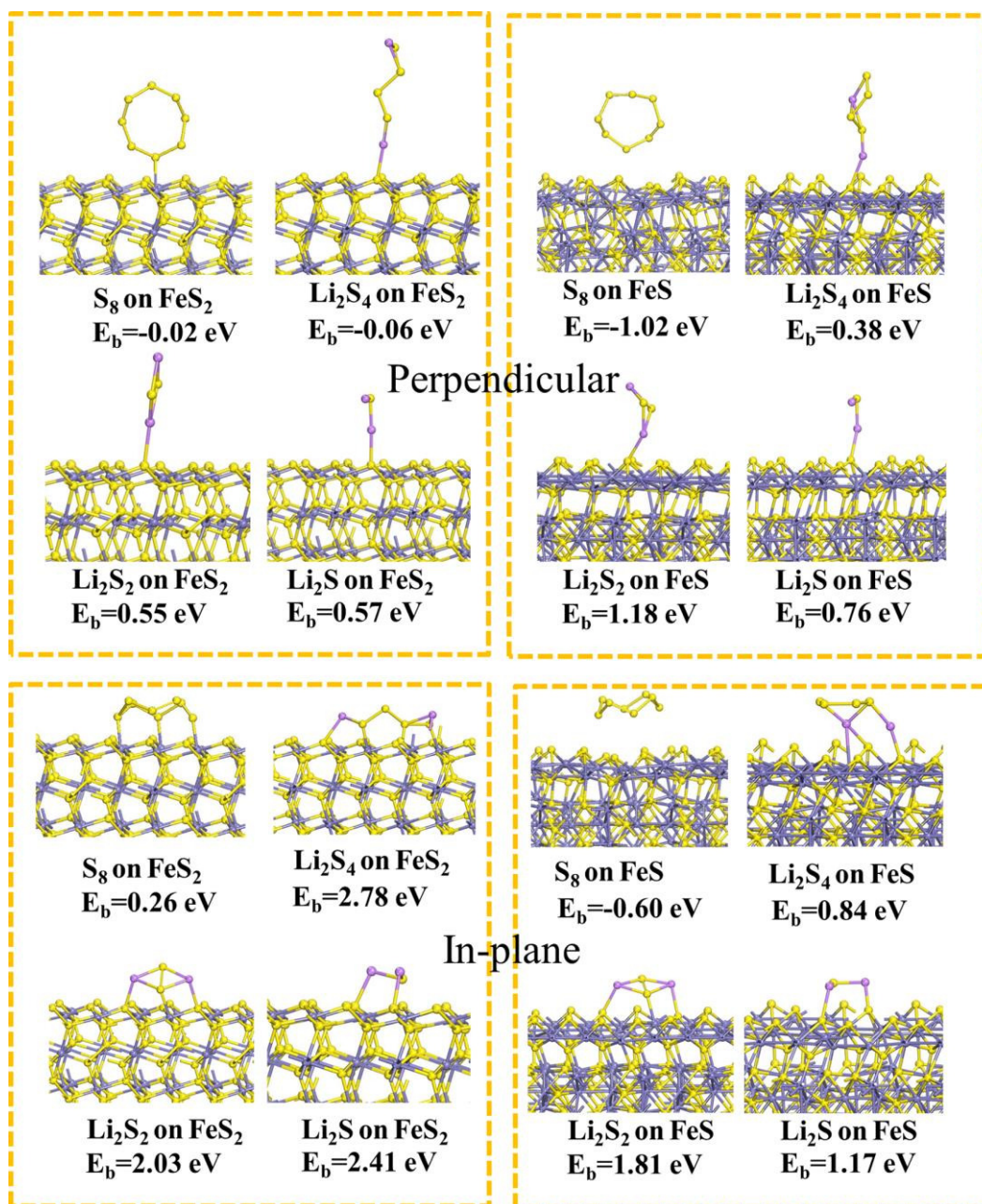


Figure S8. Optimized geometries of S_8 , Li_2S_4 , Li_2S_2 and Li_2S on FeS_2 and FeS surfaces.

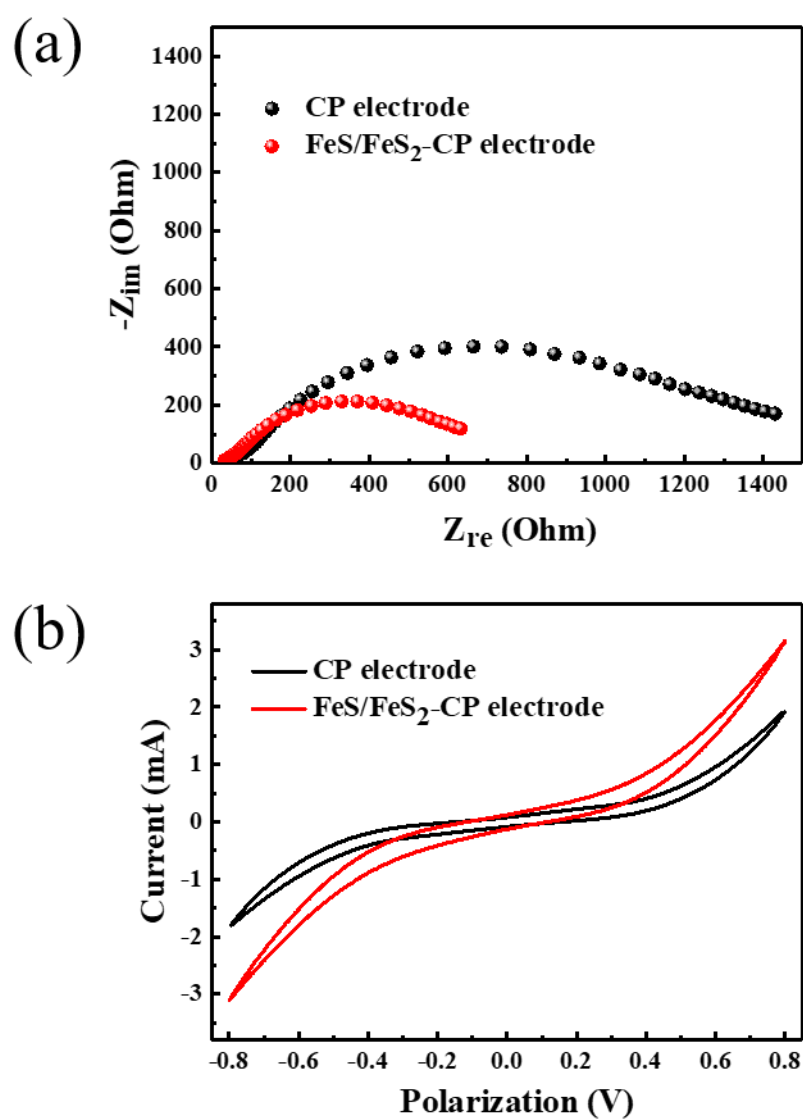


Figure S9. Electrochemical impedance spectroscopy (a) and CVs (b) of CP electrode with or without FeS/FeS₂.