Supplementary information

An in-situ encapsulation approach for polysulfide retention in lithium-sulfur batteries

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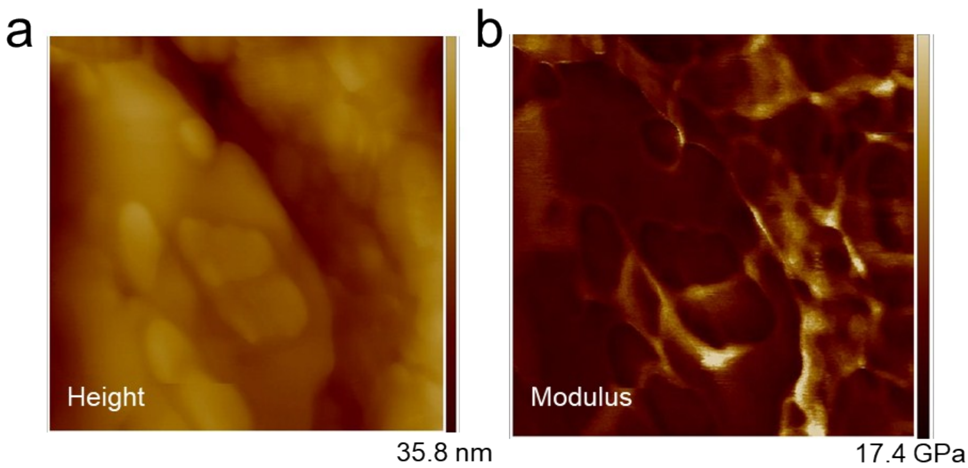

Fig. S1 The atomic force microscopy (AFM) image. (a, b) The distribution of height (a) and modulus (b). Young's modulus is calculated using a DMT model that is applied to the unloading portion of the force-separation curve[1]. The measured area is 500 nm x 500 nm.

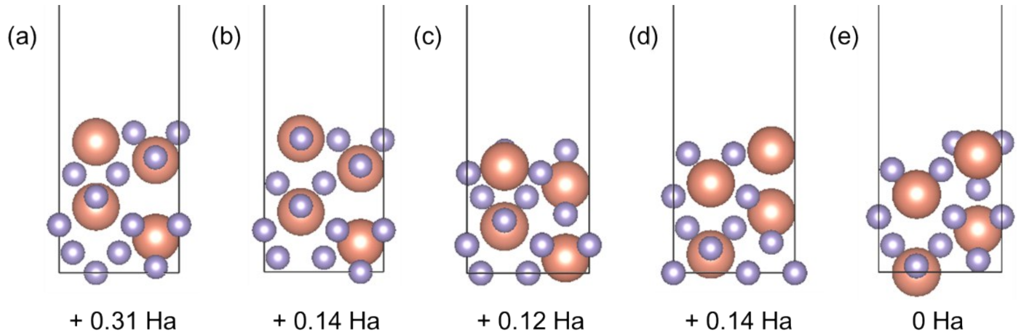

Fig. S2 The optimized atomic structures and relative energies of SbF_3 (100) surface with different terminations.

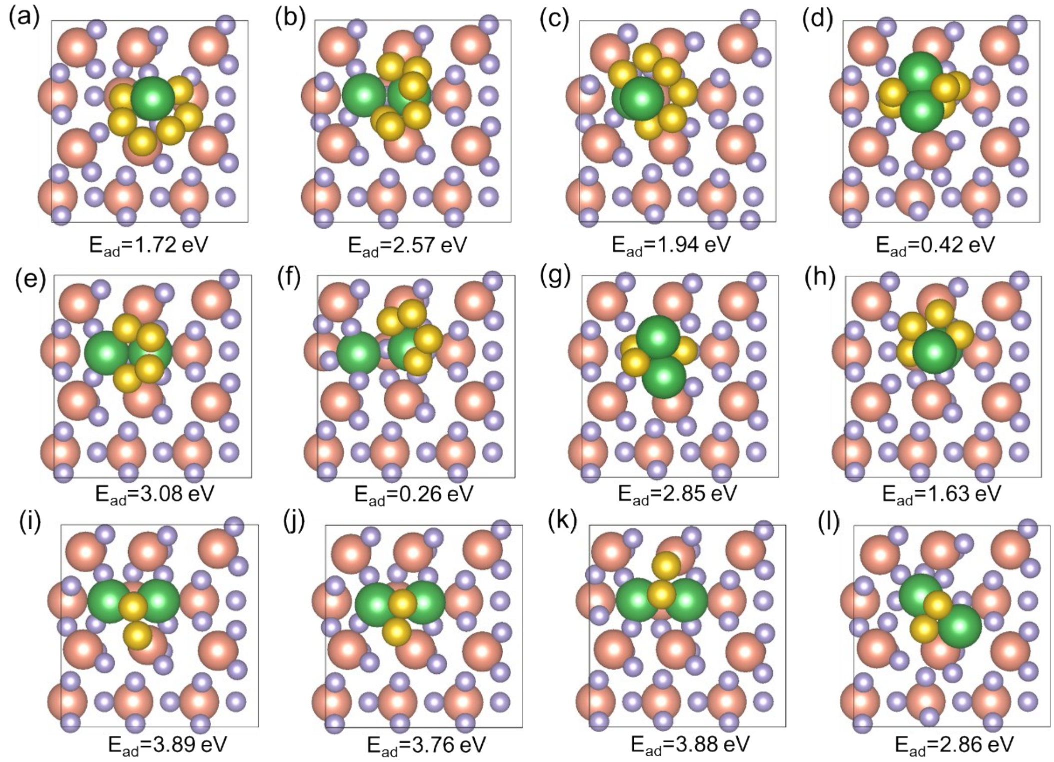

Fig. S3 (a-d) The representative structures of Li_2S_6 adsorbed on SbF_3 (200) surface; (e-h) the representative structures of Li_2S_4 adsorbed on SbF_3 (200) surface; (i-l) the representative structures of Li_2S_2 adsorbed on SbF_3 (200) surface.

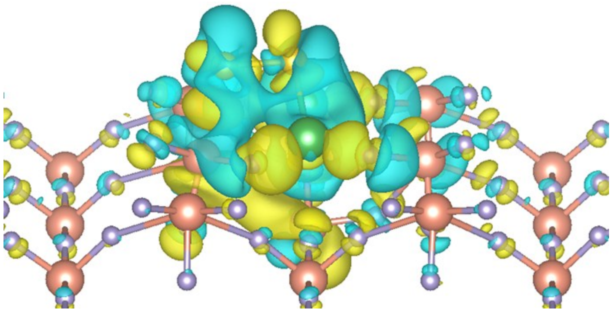

Fig. S4 Charge density difference plots showing the adsorption of Li_2S_2 on the substrate of SbF_3 (200).

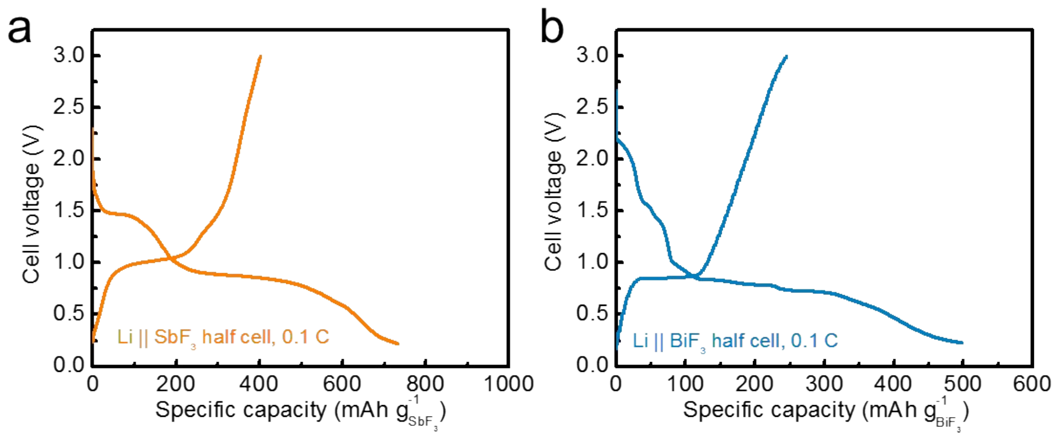

Fig. S5 Lithiation/delithiation voltage profiles for SbF_3 and BiF_3. SbF_3 starts to be lithiated below 1.5 V (versus Li), outside the voltage window of Li-S battery.

Supplementary Note 1

To fabricate the electrode, SbF_3 or BiF_3 was mixed with Super P and PVDF with a mass ratio of 8:1:1 to form a homogeneous slurry in NMP. The slurry was blade-casted on Al foil and dried at 110 °C. The SbF_3 or BiF_3 electrode (12 mm in diameter, 0.8 mg cm^{-2} active material loading) was paired with a Li foil anode (16 mm in diameter). One Celgard 2500 separator was set in between the electrodes. 100 μL classical liquid electrolyte (1.0 M LiTFSI in DOL/DME, 1.0 wt% $LiNO_3$) was added.

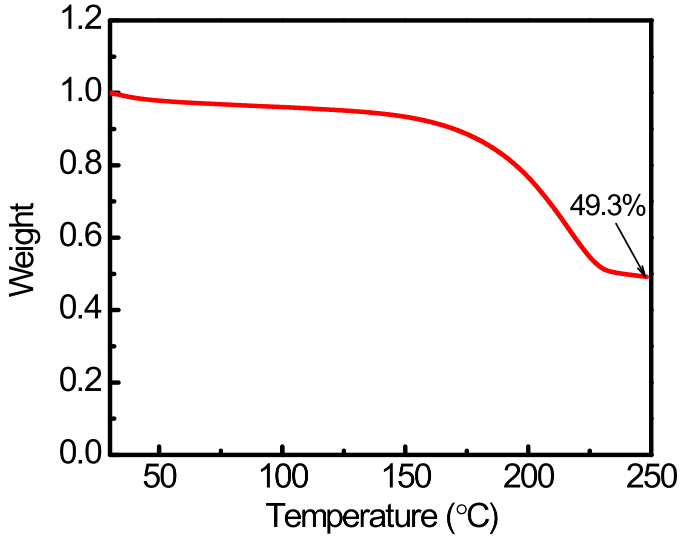

Fig. S6 TGA analysis of the S/C composite.

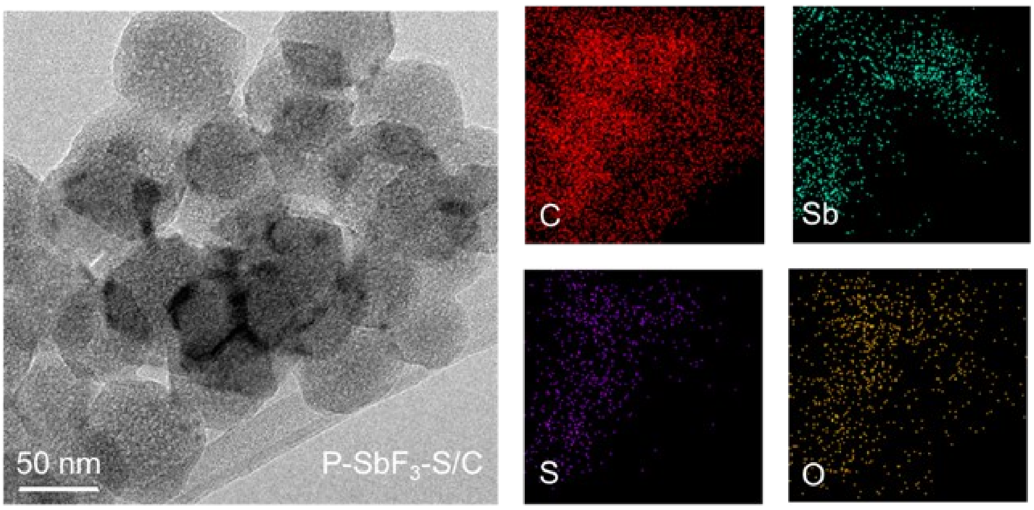

Fig. S7 TEM/EDX images of P-SbF_3-S/C, the TEM image can be also found in Fig.

4b.

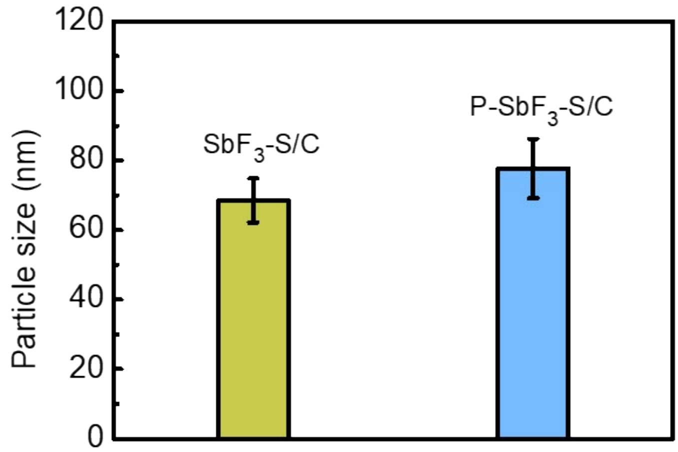

Fig. S8 The average particle size of SbF_3-S/C and P-SbF_3-S/C (number of samples:8).

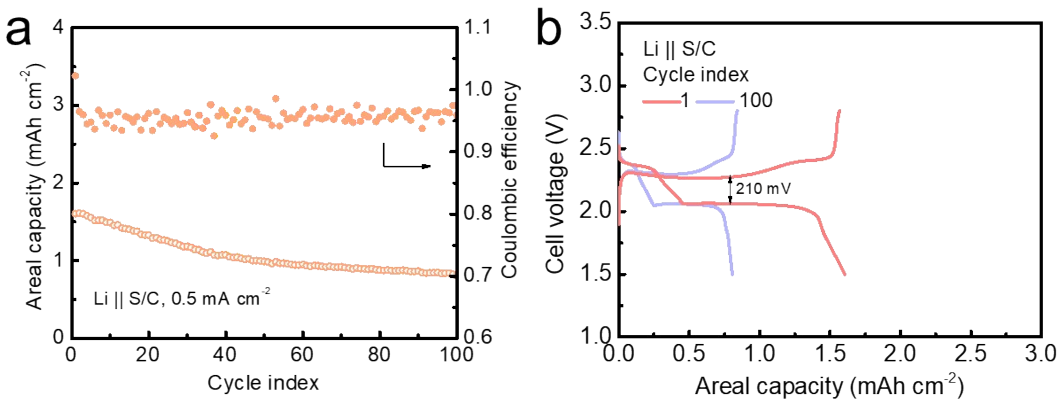

Fig. S9 (a) Cyclability of the Li-S battery with the bare S/C electrode, and (b) the corresponding voltage profiles.

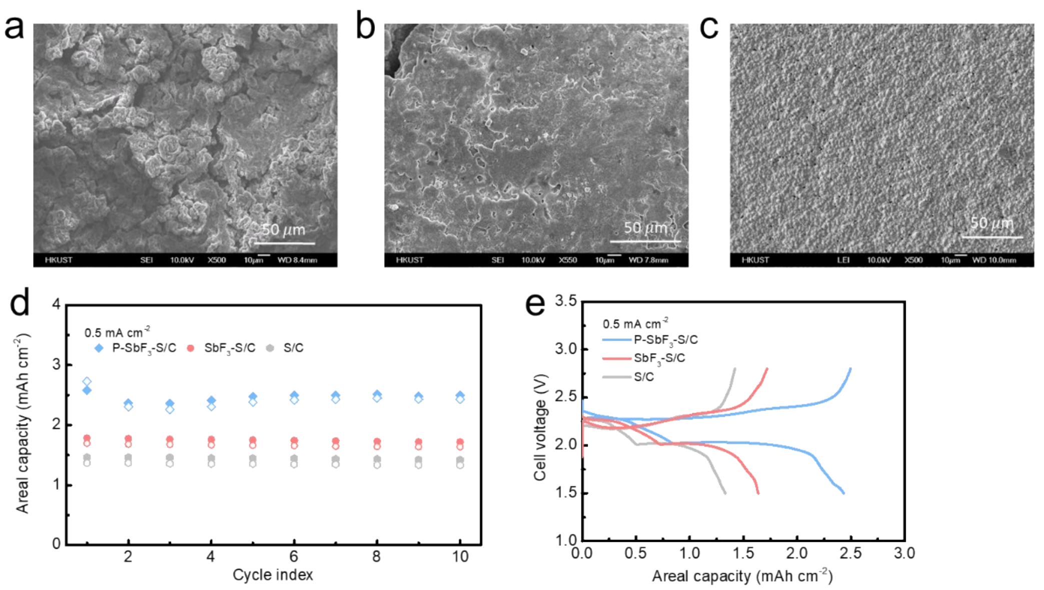

Fig. S10 (a-c) Surface SEM images of the cycled Li metal anodes from half cells with S/C (a), SbF_3/S/C (b), or P-SbF_3-S/C (c) cathode, respectively. (d, e) Cyclability of the Li-S battery with these three electrodes, and the corresponding voltage profiles at the 10^{th} cycle. The three half cells were cycled for 10 times respectively at 0.5 mA cm^{-2}, and unpacked at the charged state for characterizations.

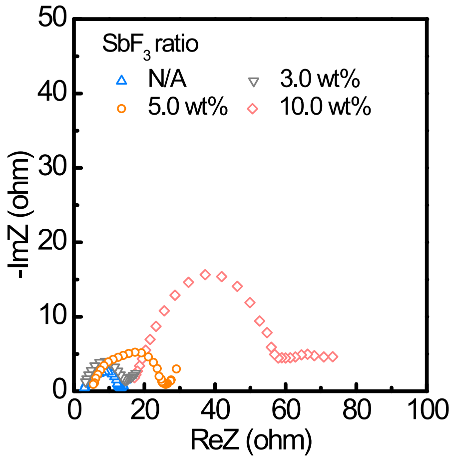

Fig. S11 Electrochemical impedance spectroscopy (EIS) of charged Li || P-SbF_3-S/C half cell with different ratios of SbF_3.

References

1. T. Young, M. Monclus, T. Burnett, W. Broughton, S. Ogin and P. Smith, *Measurement Science and Technology*, 2011, **22**, 125703.