Electronic Supplementary Material (ESI) for ChemComm.
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Electronic supplementary information

Enhanced lithium polysulfide adsorption on iron oxide modified separator for Li-S batteries

Chemicals:

All reagents were of analytical grade and used without further purification. The glucose and ferric nitrate ($Fe(NO_3)_3$) were purchased from Macklin Biochemical Co., Ltd.

Synthesis:

4.5 g of glucose was added to 30 ml of deionized water and stirred for half an hour. The solution was transferred into a 50 mL autoclave and reacted in an oven towel at 180°C for 5 h to obtain a dark brown precipitate. After washing and drying, the sample of carbon spheres was obtained.

Carbon spheres and ferric nitrate (mass ratio 1:1) were added to 30 mL of deionized water, then sonicated for half an hour and stirred for 1 hour, finally dried at 80°C for 12 h. The precipitate was calcined under air atmosphere at a temperature of 700°C for 2 h to obtain the red-brown powder of IO-700. By varying the calcination temperature in the above preparation, comparison samples of IO-600 and IO-800 can be obtained.

Characterization:

The XRD patterns of catalysts were recorded on an X-ray diffractometer (D/max 2550) with Cu Kα radiation at a scan rate of 10° min^{-1} from 10° to 80°. The HRTEM operated at 200 kV and the corresponding EDS were acquired by Titan 80-300 instrument (300 kV). The XPS was performed by the Thermo Fisher Escalab 250Xi XPS instrument with Al Kα as emission source. The spectra were calibrated with the position of C 1s peak (284.8 eV). The thermal gravimetric analyzer (TGA, Netzsch

STA409PC) was applied to detect the sulfur content.

Electrochemical measurements:

In a typical procedure, a mixture of oxide catalyst, carbon black (CB) and polyvinylidene difluoride (PVDF) powder (8:1:1 by mass) was dispersed in N-Methylpyrrolidone (NMP) solvent. The mixture stirred for 0.5 h and then scraped directly onto commercial PP (Celgard 2400). The obtained modified separator (IO-700@PP) was dried in a vacuum oven at 60°C for 12 h. The modified separators were then cut into discs with a diameter of 19 mm and a corresponding area mass of about 0.24 mg cm^{-2}. Dispersion of a mixture of S, carbon black and PVDF) in NMP solvent to form a slurry, which is then scraped onto aluminium foil and dried in an oven for 12 hours to obtain the C/S cathode with an area mass of 1 mg cm^{-2}. The coin cell (type CR2032) was constructed using modified separator, DME/DOL (1:1, vol%) electrolyte with 1.0 M LiTFSI and 0.2 M $LiNO_3$, and a lithium metal electrode and C/S cathode in an argon-filled glove box. The cells were tested in galvanostatic measurements in a voltage range from 1.7 to 2.8 V by NEWARE testing system.

Li_2S_6 adsorption test: The Li_2S_6 solution was prepared by mixing Li_2S and S powder with a molar ratio of 1:5 into the mixed solvent 1,2-dimethoxyethane (DME) and 1,3-dioxolane (DOL/DME, 1:1 by volume) with vigorous stir in an argon-filled glove box. Then the samples of IO-600, IO-700 and IO-800 (10 mg) were added into the 0.01 M Li_2S_6 solution. The solution was standing for 6 h to estimate the adsorption

capabilities of each coating material.

Density functional theory (DFT) calculations

The density functional theory (DFT) with project augmented wave method (PAW) implemented in the Vienna ab initio Simulation Package (VASP) was used to perform the calculations. The exchange and correlation energy was achieved using the Perdue-Burke-Enzerhof (PBE) version within the generalized gradient approximation (GGA). In order to avoid possible interactions between the slabs induced by periodicity, a reasonable vacuum was set at 15 Å in the z-direction. The Brillouin-Zone integrations used a Gamma only k-point setup, and the plane wave adopted an energy cut-off of 450 eV. In the geometry optimization, the energy and maximum force convergence criteria were taken as 10^{-5} eV and 0.03 eV $Å^{-1}$, respectively.

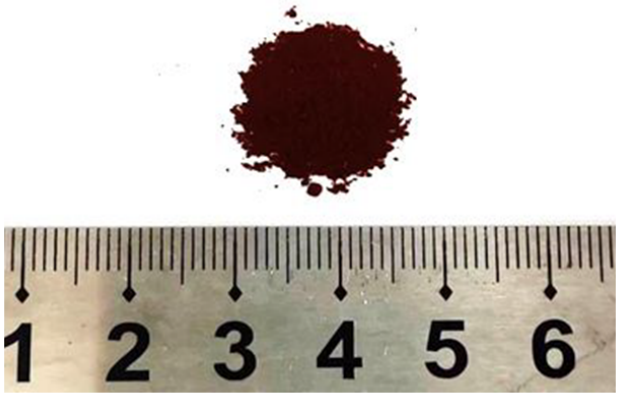

Fig. S1 The photo of IO-700 catalyst.

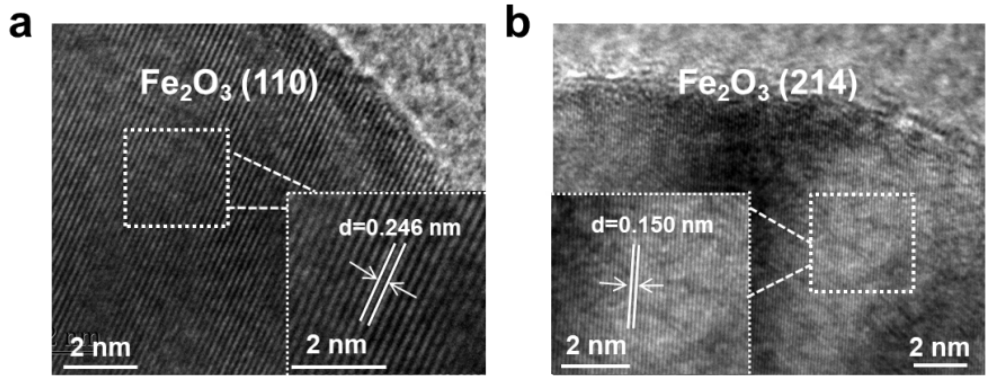

Fig. S2 HRTEM images and the corresponding lattice spacing at the selected area of Fe_2O_3 exposed with (a) (110) and (b) (214) facets.

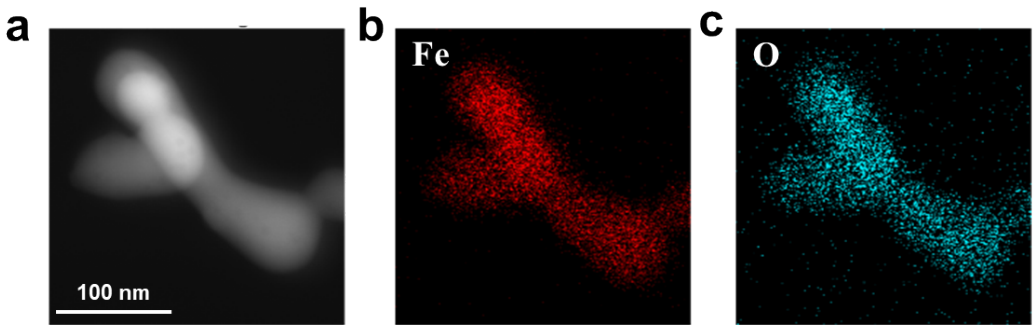

Fig. S3 The elemental mapping images of IO-700.

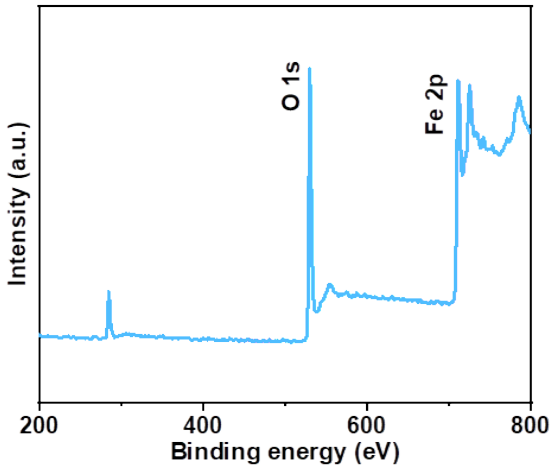

Figure S4. The full XPS profile of IO-700.

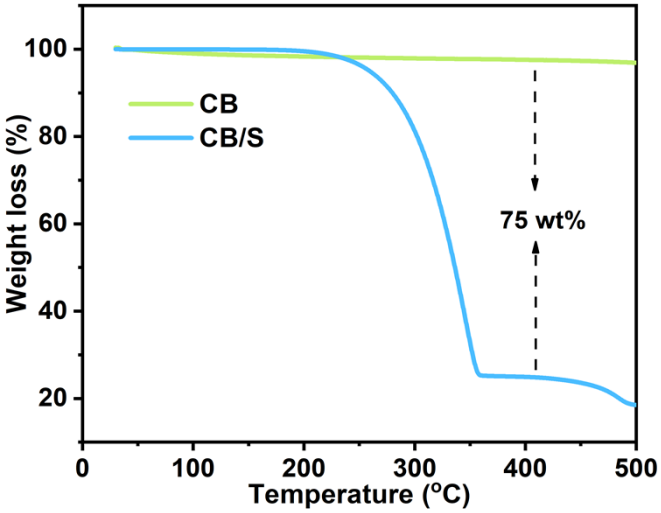

Fig. S5 TGA curves of CB and CB/S.

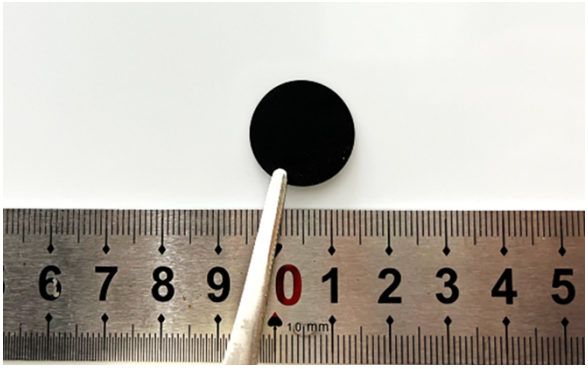

Fig. S6 The image of sulfur cathode.

Fig. S7 The image of coin Li-S battery.

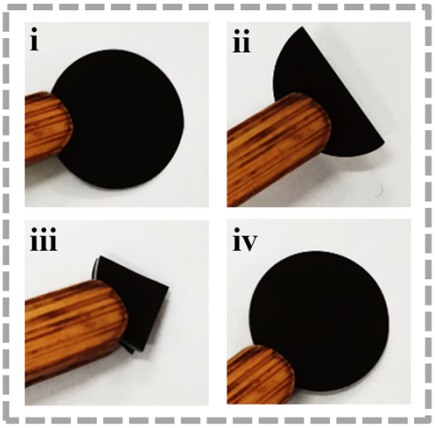

Fig. S8 (a) Optical images of IO-700 modified separator (black) under various mechanical deformations. (i) flat, (ii) bend, (iii) fold and (vi) recover.