Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Supporting Information for High Performance Li-S Battery Based on Amorphous NiS_2 as the Host Material for the S Cathode

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S1 Detail of Experiment:

Synthesis of S@a-NiS_2, a-NiS_2 and c-NiS_2

The S@a-NiS_2 composite was obtained through a simple solution process at room temperature. Na_2S_8 was synthesized through the reported method under the protection of Argon, 1 g Na_2S and 20 g S was mixed, to make sure that the S was excessive. The mixture was further transferred into 200 mL ethanol and heated at 50 ℃ for 24 hours. Then the obtained Na_2S_8 ethanol solution was dripped into 50 mL 0.1M $NiCl_2$ ethanol solution at room temperature and the obtained black precipitate was separated and repeated washed by ethanol.

The a-NiS_2 was obtained by repeated wash the S@a-NiS_2 composite with CS_2, and heated at 60 ℃ for 24 hours.

The c-NiS_2 was obtained through the same process of a-NiS_2 but the reaction temperature of the formation of NiS_2 was 60 ℃.

Preparation of the S cathode

The S cathode was prepared by mixing the S@a-NiS_2 composite with carbon black and poly(vinylidenedi fluoride) (PVDF) at a weight ratio of 8:1:1 and loading the prepared mixture on a piece of aluminum foil, areal S mass loading was ~1 mg/cm^2.

Assemble of Li-S coin cells.

2032-type coin cells were fabricated in an Ar-filled glove box (MIKROUNA, China) using a Li foil as the counter electrode, a cellgard 2340 micro-porous membrane as the separator, and lithium bis(trifluoromethanesulfonyl)imide (0.8 M) and $LiNO_3$ (0.2 M) in 1,2-dimethoxyethane and 1,3-dioxolane (1:1 vol%) as the electrolyte.

Characterization and measurements

The S@a-NiS_2, a-NiS_2 and c-NiS_2 was characterized by X-ray diffraction (XRD) (D/MAX 2500/PC), XPS (250 Xi) and thermogravimetric analysis (TGA) (TG 209 F3). The morphology of the samples was characterized by TEM (FEI F20) and SEM (SUPRA 55). The coin cells were cycled from 1.8 to 3.0 V versus Li^+/Li with a multichannel battery tester (NEWARE BTS-5V20 mA). Specific charge–discharge capacities were calculated based on the mass of S.

S2 The Ni 2p core-level XPS spectrum.

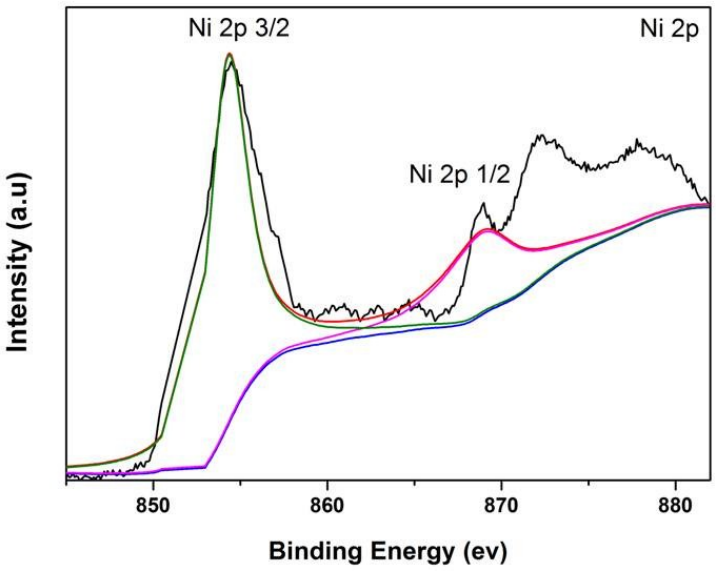

Figure S1 The Ni 2p core-level XPS spectrum.

S3 EDS of the amorphous NiS_2 in the HRTEM image.

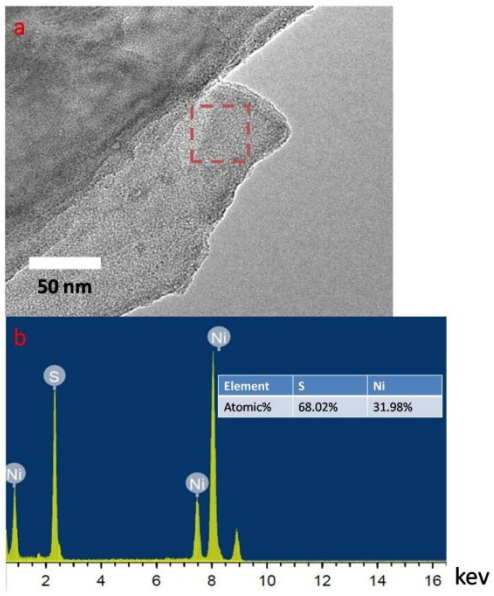

Figure S2 HRTEM of amorphous NiS_2 (a) and EDS of the marked position in figure S3a (b).

S4 SEM of the S@NiS_2 composite, amorphous NiS_2 and crystal NiS_2.

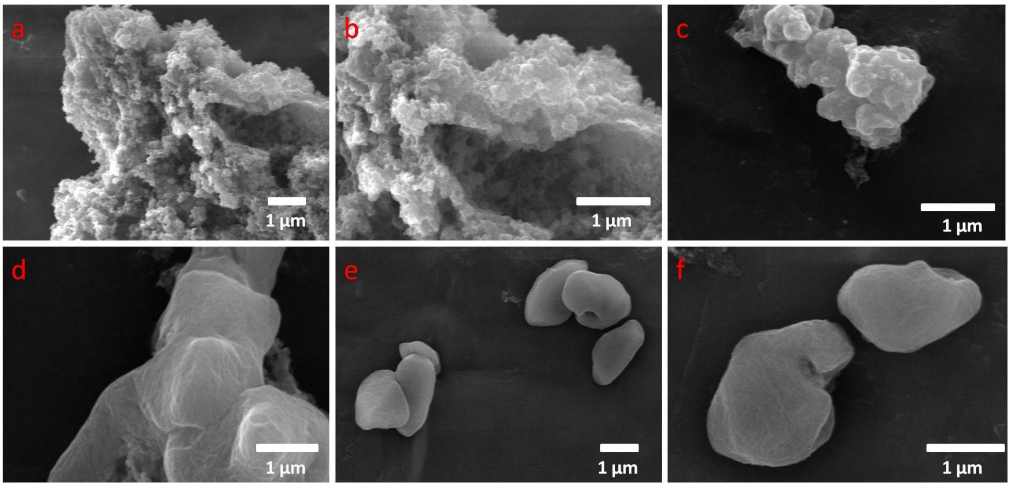

Figure S3 SEM of the S@NiS_2 composite (a, b), amorphous NiS_2 (c, d)and crystal NiS_2 (e, f).

S5 TGA curve of the S@a-NiS_2 composite measured in a nitrogen environment.

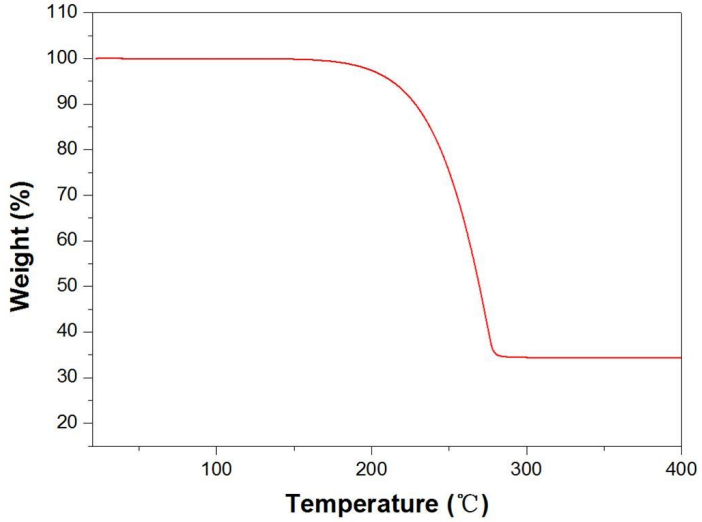

Figure S4 TGA curve of the S@a-NiS_2 composite measured in a nitrogen environment.

S6 Charge and discharge curve of Battery with only a-NiS_2 as the cathode material.

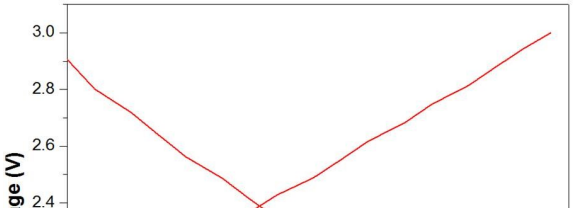

Figure S5 Charge and discharge curve of Battery with only a-NiS_2 as the cathode material. The electrolyte was lithium bis(trifluoromethanesulfonyl)imide (0.8 M) and $LiNO_3$ (0.2 M) in 1,2-dimethoxyethane and 1,3-dioxolane (1:1 vol%).

S7 Charge and discharge curve of Battery with only a-NiS_2 as the cathode material.

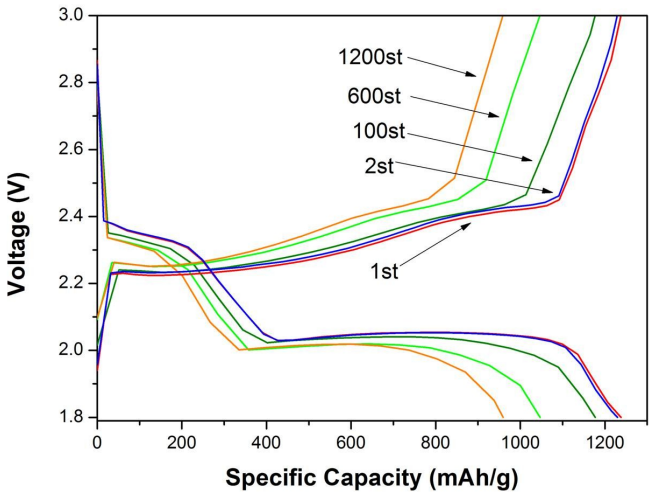

Figure S6 The voltage profiles during the 1200 cycles (Fig. 5a), containing 1st, 2nd, 100th, 600th, and 1200th.

S8 XRD spectrum of crystal NiS_2 obtained at 60 ℃.

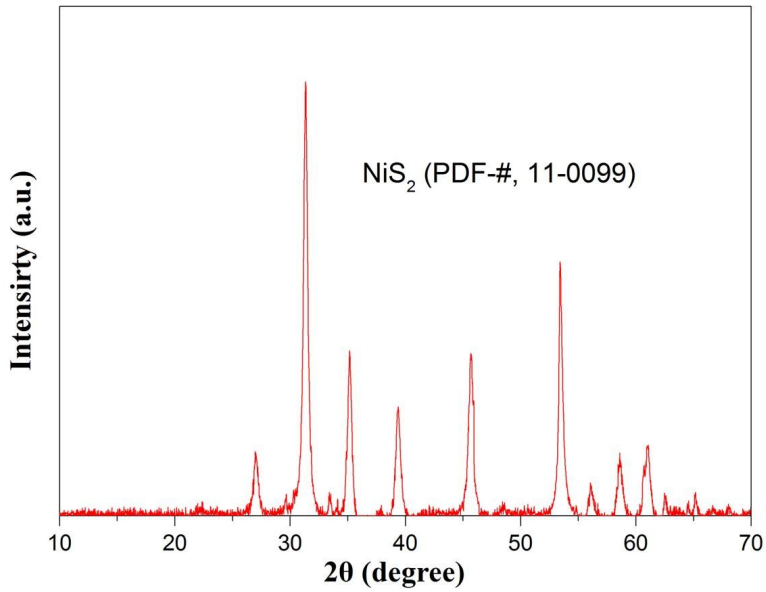

Figure S7 XRD spectrum of crystal NiS_2

S9 Electrochemical impendence of a-NiS2 battery and active carbon battery.

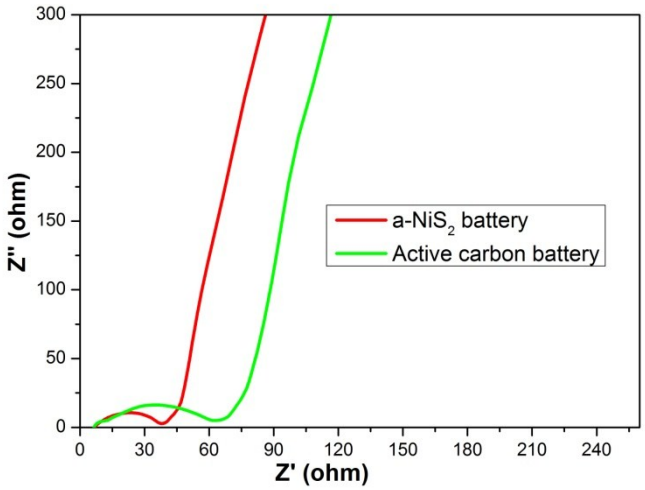

Figure S8 Electrochemical impendence of a-NiS2 battery and active carbon battery.