Electronic Supplementary Information

Facile Synthesis of Sulfide $Bi_{13}S_{18}I_2$ as a promising Anode Material for Lithium ion Battery

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Materials and Methods

2.1.1 The fabrication of $Bi_{13}S_{18}I_2$ (BSI) powders

Typically, $Bi(NO)_3$~$5H_2O$, NaI, and CH_4N_2S were dissoved to glycol and deionized water by weight ratio. respectively. Then the solution was put into a high pressure reactor at 120℃ for 12 h. After the reaction was over, the black precipitate obtained was filtered and washed by centrifugation with deionized water and anhydrous ethanol several times and dried in a drying oven at 80 °C for 12 hours to obtain $Bi_{13}S_{18}I_2$. All chemicals were purchased from Aladding without further purification.

2.1.2 Preparation of graphene/BSI composite

Graphene and BSI were added to ethanol and deionized water with different weight ratios. After acoustic wave treated for 30 minutes, a uniform solution was formed, and then the reaction was carried out in a high-pressure reactor. The material obtained by the reaction was cleaned several times with water and alcohol, and dried in a drying oven for 12 h to get the final graphene/BSI. To obtain the best electrochemical performance, the graphene content was 100 mg, 150 mg and 200 mg, respectively. The

optimized 150 G/BSI samples are characterized in detail. To easy remember the samples, the BSI with different graphene content were denoted as 100G/BSI, 150 G/BSI, 200 G/BSI.

2.2 Material characterization

The morphologies of the samples were characterized by field emission scanning electron microscopy (FE-SEM, JEOL7800F) and transmission electron microscopy (TEM, JEOL 2010F). The crystal structure of the composite was analyzed by X-ray diffraction (XRD), SDT Q600. Raman spectra were taken on a DXR Raman microscope (Thermal Sciences Corporation, wavelength 532 nm). X-ray photoelectron spectroscopy (XPS) analysis was performed on an ESCALAB 250 Thermo Fisher Scientific.

2.3 Electrochemical measurements

The electrode material is obtained by conventional slurry coating method. The original synthetic material, acetylene black, adhesive according to the weight ratio of 8:1:1 mixed, after stirring for 2 h drops of n-methylpyrrolidone, to get a uniform mixture, after stirring for 24 h the mixture evenly coated on copper foil, in 80 ℃ blast drying oven after roller press, and then in 60 °C vacuum drying, A slurry containing about 1.0~1.5 mg cm−2 active substance is obtained. The button half battery (CR2025) is assembled in an argon filled glove box (H_2O, O_2 < 0.1 ppm). The reference electrode and opposite electrode are lithium foil. NEWARE CT-3008 is used to obtain the charge-discharge curve with current density of 0.5~ 0.05 A/g and voltage range of 0.01 ~ 3.0 V. The BSI samples with different graphene addition are denoted as BSI, 100 G/BSI, 150G/BSI, and 200 G/BSI, respectively.

Figures

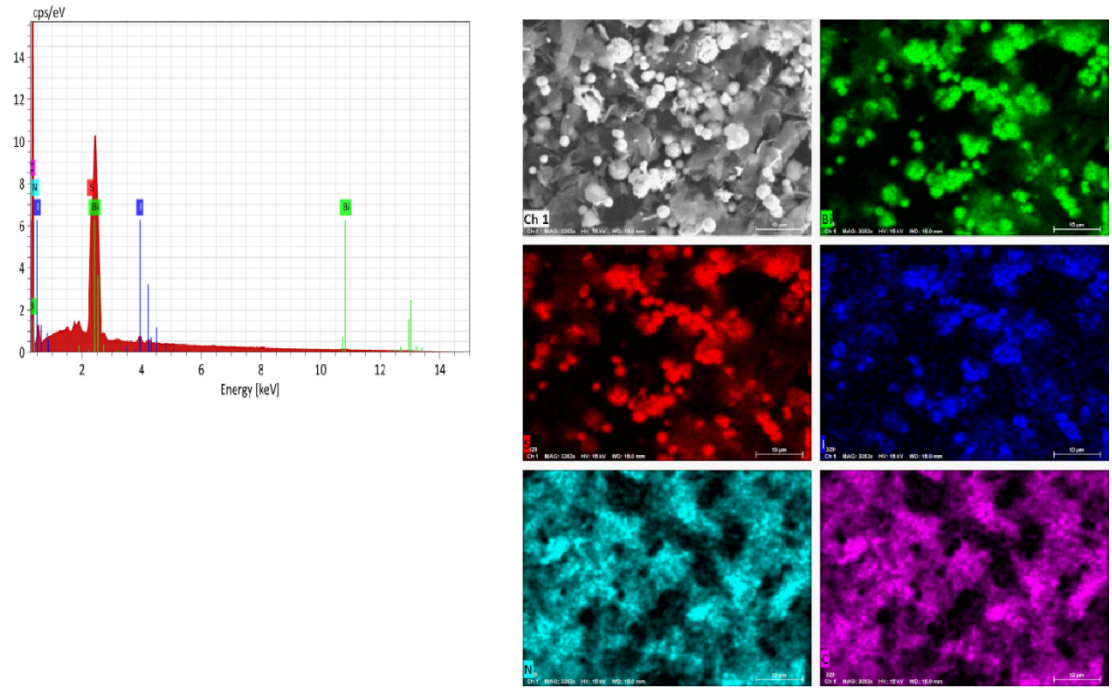


Fig. S1 EDS mapping of the 150 G/BSI.

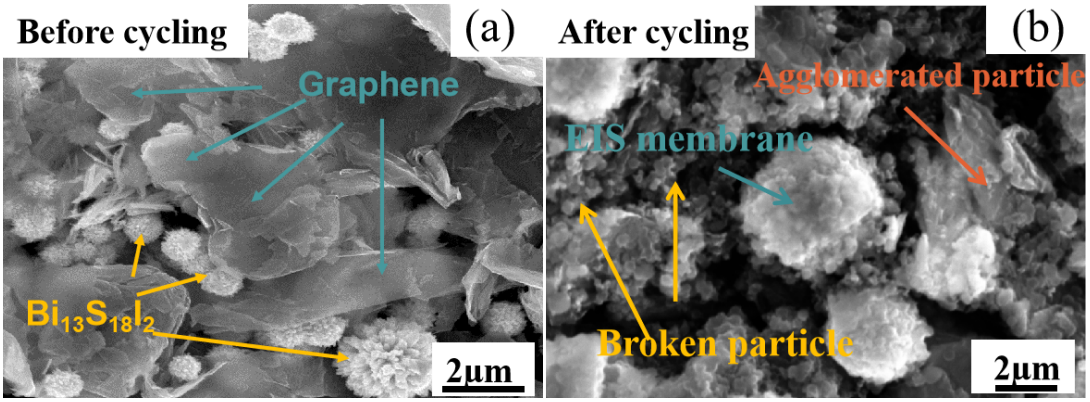


Fig. S2 (a) FE-TEM image of the 150 G/BSI electrode before cycling; (b) FE-TEM images of the 150 G/BSI electrode after 500 cycles.

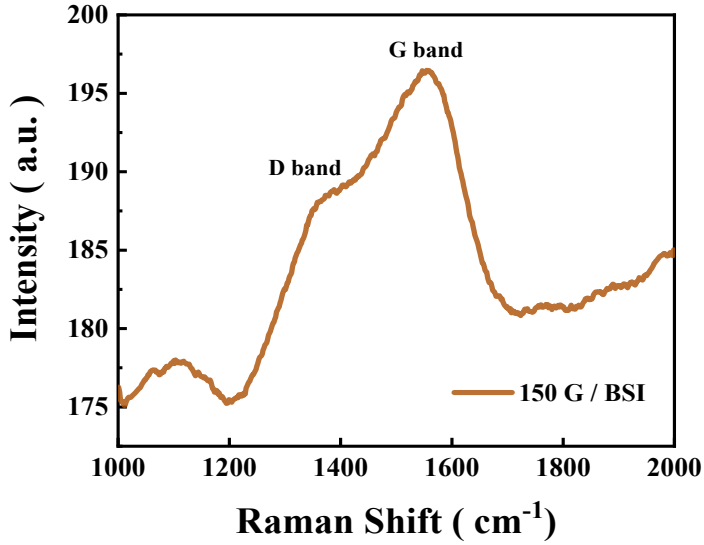


Fig. S3 Raman spectrum of the 150 G/BSI.

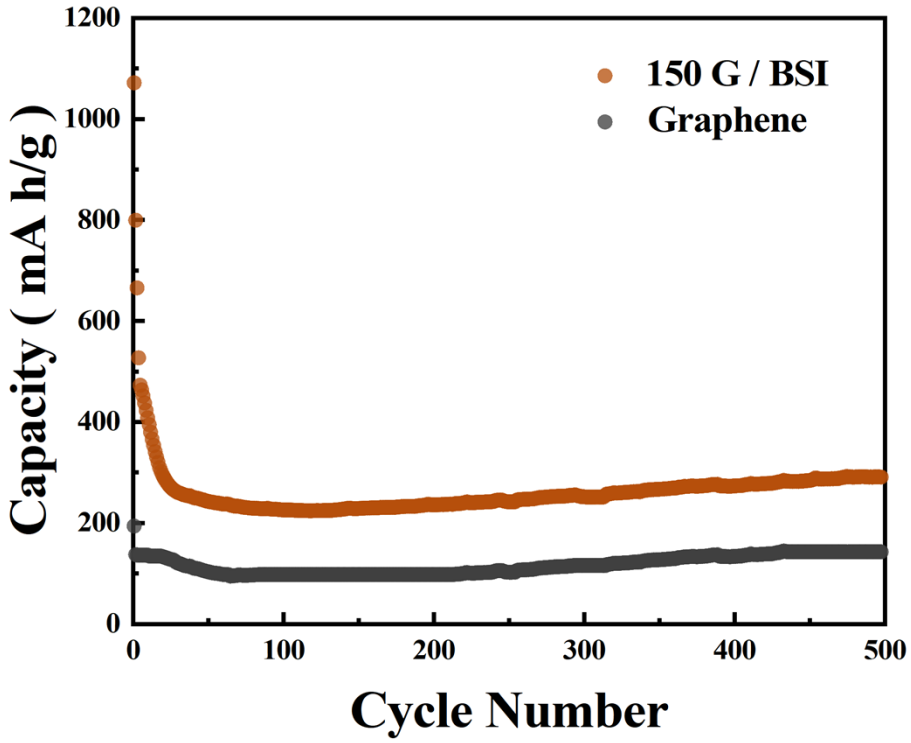


Fig. S4 Long Cycle Performance of Graphene and 150 G / BSI at 0.5 A/g

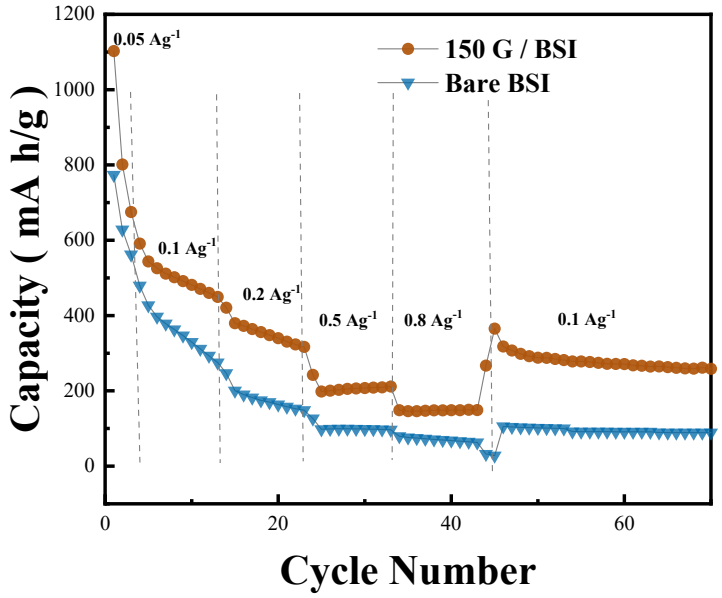


Fig. S5 Rate performance at different current densitieso of Bare BSI and 150 G/BSI.

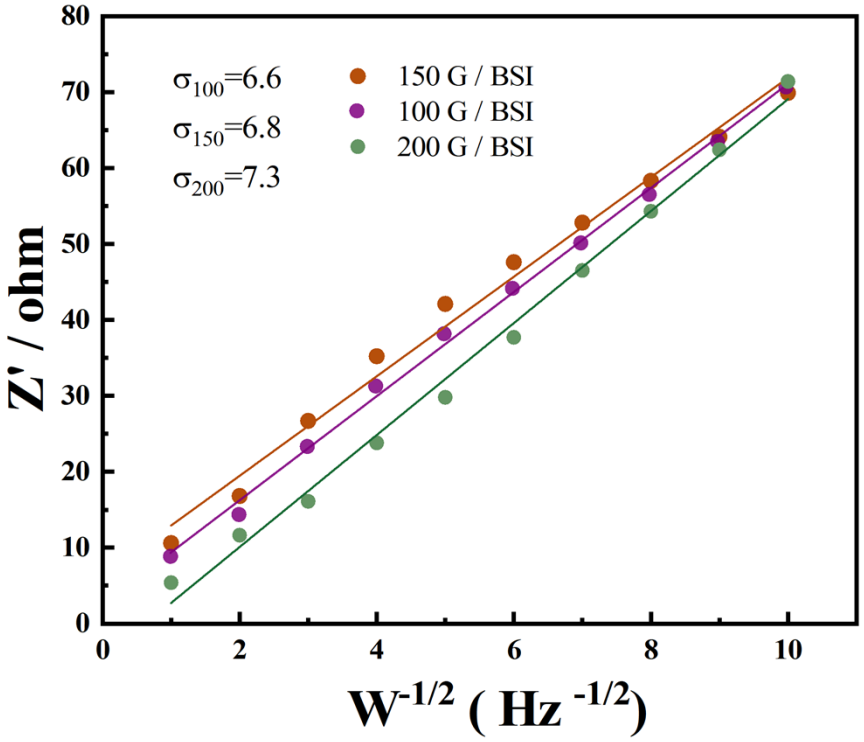


Fig. S6 Relation of Z'-$x^{-1/2}$ curves in the low-frequency region for the 100 G / BSI, 150 G / BSI, 200 G / BSI

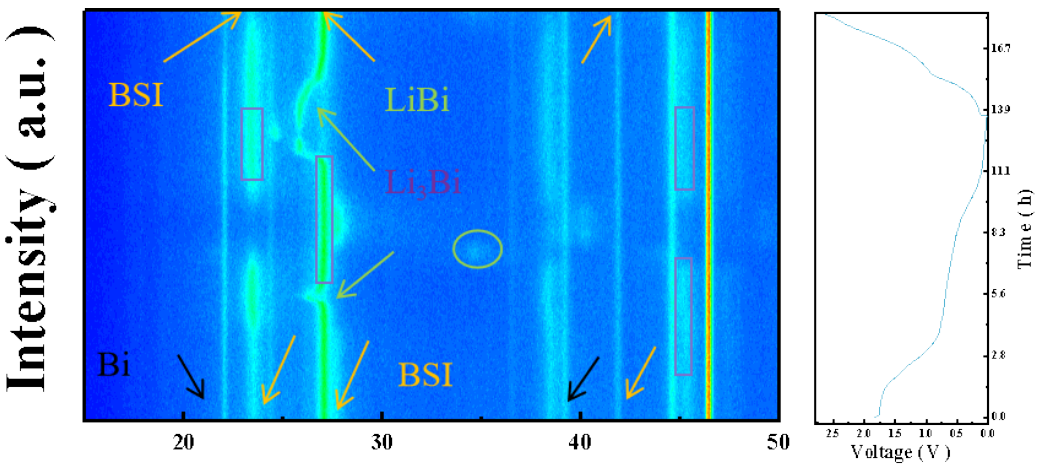


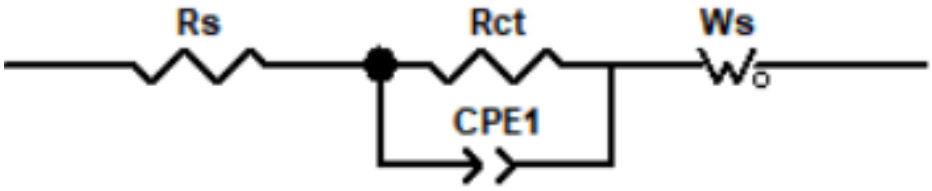
Fig. S7 In situ XRD patterns of the 150 G/BSI electrode during the first cycle and the corresponding discharge and charge curves.

Fig.S7 shows the reaction mechanism of the 150 G/BSI composite could be described as follows:
In the discharge process

$$Bi_{13}S_{18}I_2 \xrightarrow{+Li} 13Bi + 18Li_2S + 2LiI \xrightarrow{+Li} 13LiBi$$

In the charge process

$$Li_3Bi \xrightarrow{-Li} LiBi \xrightarrow{-Li} Bi$$



	Re/Ω	Rct/Ω
100 G /BSI	9.89	108.1
150 G /BSI	6.85	104.6
200 G /BSI	11.55	111.2

Table S1 Equivalent electrical circuit and resistance values (in Ω)