Supporting Information

In situ chemistry-encapsulated controlled SnS_2 nanocrystal composites for durable lithium/sodium-ion batteries

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Experimental Section

The Preparation of C-SnS_2@rGO-X (X=0.1, 0.2, 0.4), SnS_2@rGO and SnS_2.

First, 0.1 g of GO was dissolved into a solution consisting of water (40 mL) and alcohol (20 mL) by ultrasonication of 2 h to obtain the GO dispersing solution. After that, various amounts of glucose (*i.e.* 0.1, 0.2 and 0.4 g), 0.16 g NaOH, 0.71 g $SnCl_4 \cdot 5H_2O$ and 1 g thiourea were added to the above solution, then stirred continued for 12 h. The resulted solution was injected into a 100 mL Teflon autoclave and was kept at 180 ^oC for 12 h. The C-SnS_2@rGO-X (X=0.1, 0.2, 0.4) was washed with deionized water and collected by centrifugation, and then dried at 60 ^oC. For comparison, the SnS_2@rGO was prepared without adding glucose; similarly, SnS_2 was prepared without adding rGO and glucose.

Characterization of Materials.

X-ray diffractometer (XRD) was performed on a Rigaku SmartLab X-ray diffractometer with Cu Kα radiation. Raman spectra were obtained with a JY HR-800 Lab Ram confocal Raman microscope. Scanning electron microscopy (SEM, XL 30 ESEM-FEG, FEI Company) and transmission electron microscopy (TEM) were employed to investigate the morphologies of the samples. X-ray photoelectron spectra (XPS) was tested with Mg-Kα excitation (1253.6 eV) in a VGESCALAB MKII spectrometer.

Electrochemical Characterization.

The SnS_2-based composites (80%), polyvinylidene fluoride (10%) and acetylene black (10%) were mixed in N-methyl-2-pyrrolidone, and then coated on the Cu foils as

working anodes. The mass loading of SnS_2-based composites in electrode was approximately 1.1 mg cm^{-2}. 2032-type coin cells were manufactured with 1 M $LiPF_6$ dissolved in dimethyl carbonate and ethylene carbonate (1:1 by volume).The charge/discharge measurements were carried out on a multichannel battery testing system (LAND CT2001A). The cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS) tests were measured on an electrochemical workstation (CHI 750 E).

Theoretical Calculation.

We perform first-principle calculations by using Vienna ab initio simulation package with the Perdew-Burke-Ernzerhof-type generalized gradient approximation for the exchange-correlation functional and the projector augmented wave method. All atoms are relaxed until the residual force was less than 0.01eV/Å. A 3 × 3 × 1 grid of k points and a plane-wave cutoff energy of 400 eV are used for the self-consistent calculations and charge analysis. The d2 vdW interactions are considered through all the calculations.

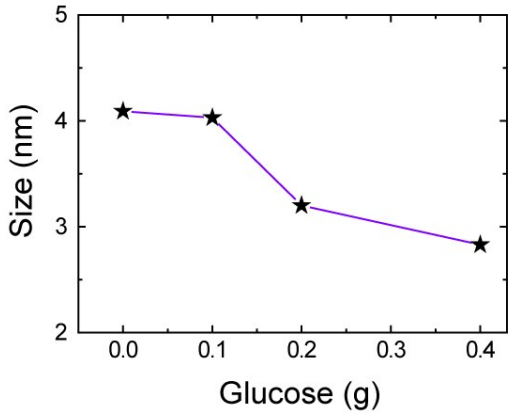

Fig. S1 The size of SnS_2 NCs under different content of glucose, demonstrating the size of SnS_2 NCs is well controlled.

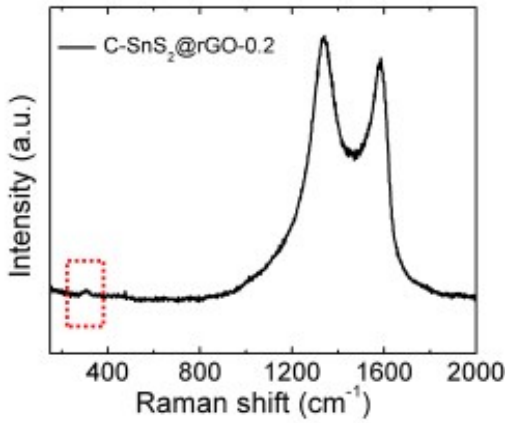

Fig. S2 The Raman spectrum of C-SnS_2@rGO-0.2, demonstrating the disordered structure of carbon.

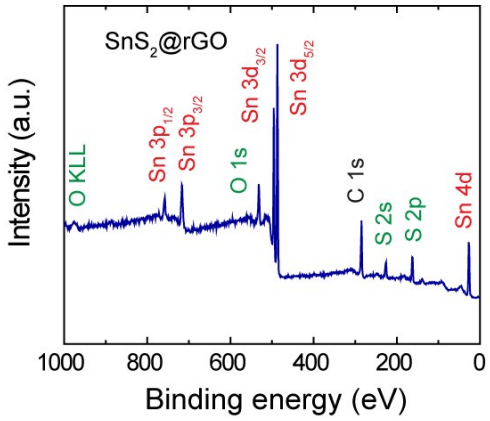

Fig. S3 XPS survey spectra of SnS_2@rGO.

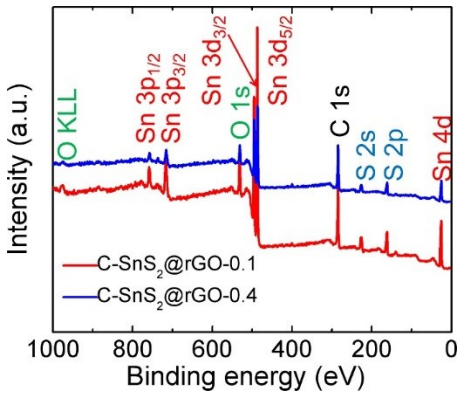

Fig. S4 XPS survey spectra of C-SnS_2@rGO-0.1 and C-SnS_2@rGO-0.4.

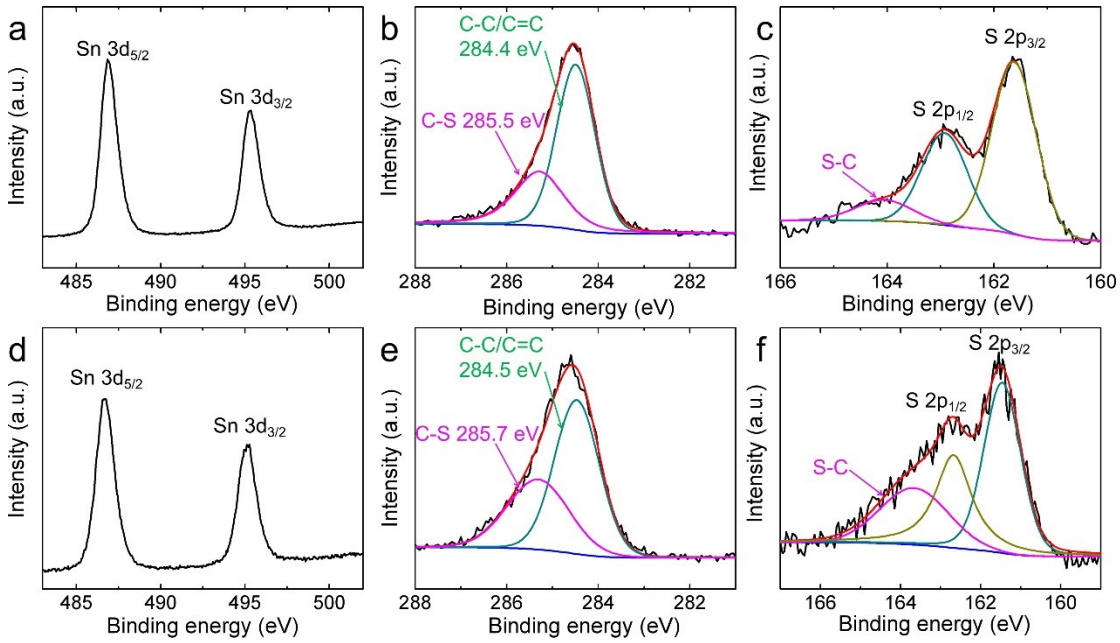

Fig. S5 XPS spectra of C-SnS_2@rGO-0.1 and C-SnS_2@rGO-0.4: (a, d) Sn 3d, (b, e) C 1s and (c, f) S 2p, revealing that the C-S bonds gradually become stronger with glucose increased in the preparation process.

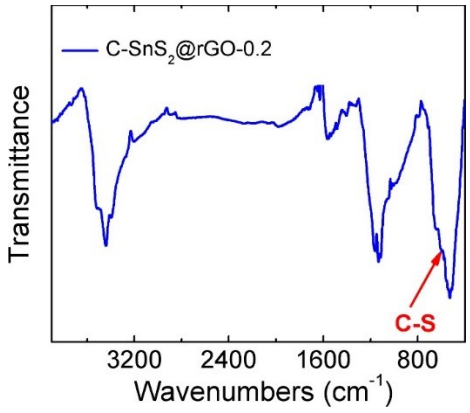

Fig. S6 FT-IR spectrum of C-SnS_2@rGO-0.2, indicating the presence of C-S bonds.

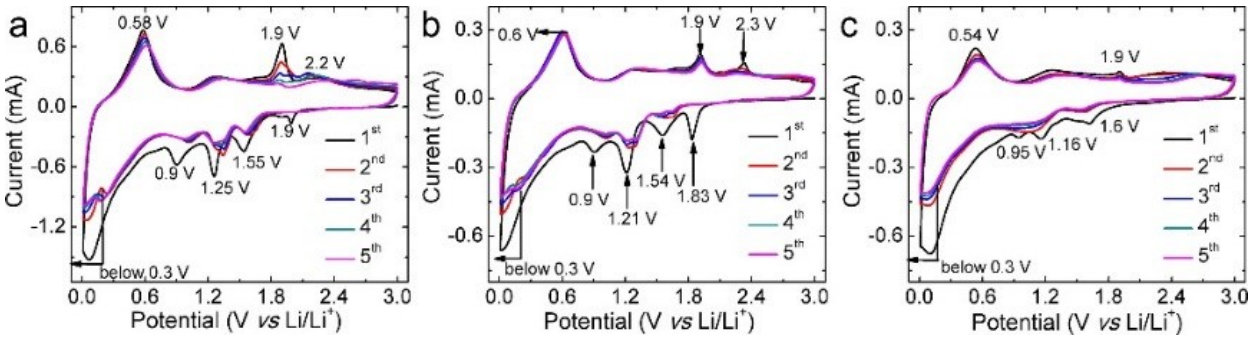

Fig. S7 CV curves of SnS_2@rGO, C-SnS_2@rGO-0.1 and C-SnS_2@rGO-0.4, exhibiting the similar electrochemical processes as C-SnS_2@rGO-0.2.

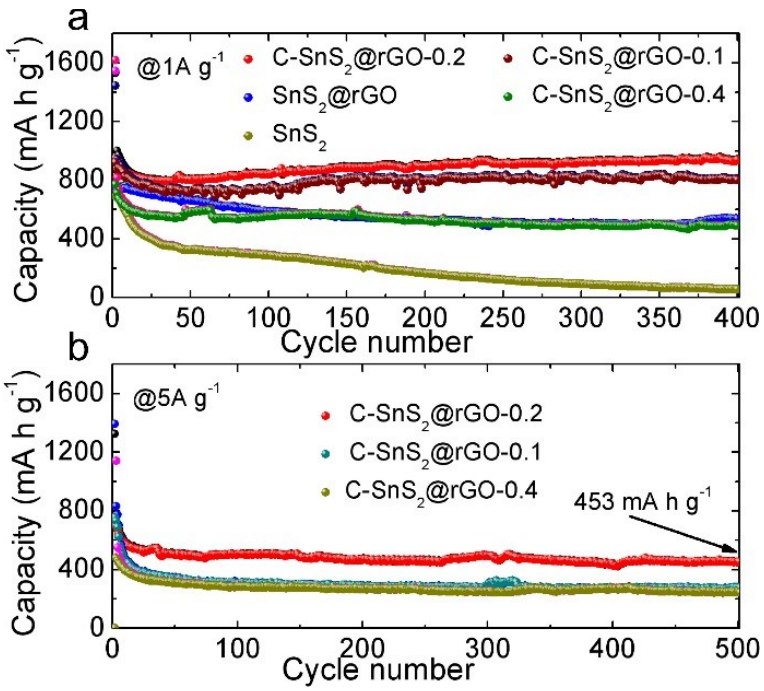

Fig. S8 The cycle performances of (a) C-SnS_2@rGO-X (X=0.1, 0.2, 0.4), SnS_2@rGO and SnS_2, (b) C-SnS_2@rGO-X (X=0.1, 0.2, 0.4) electrode.

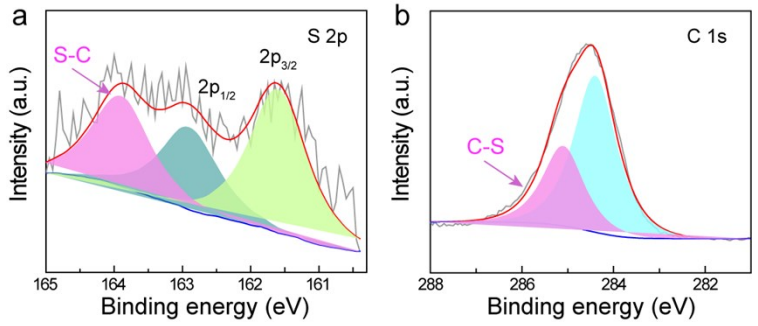

Fig. S9 The XPS spectra of C-SnS_2@rGO-0.2 (a) S 2p, (b) C 1s after 50 cycles at 1 A g^{-1}.

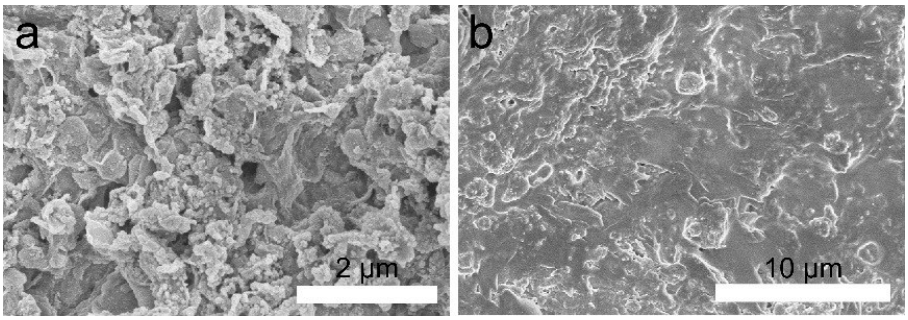

Fig. S10 SEM images of C-SnS2@rGO-0.2 after 1000 cycles, indicating the stable electrode structure.

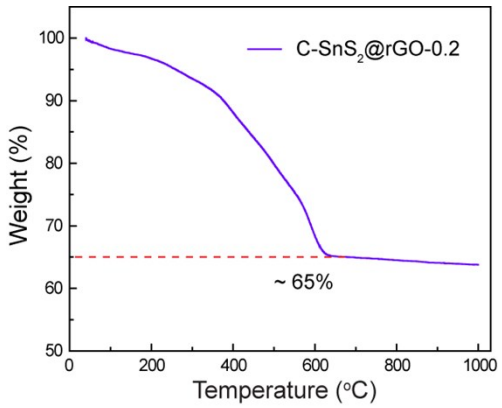

Fig. S11 The TGA curve of C-SnS_2@rGO-0.2 at atmosphere from room temperature to 1000 °C.

As shown in **Fig. S11**, the sharp weight loss before approximately 650 °C is ascribed to the conversion from SnS_2 to SnO_2 and the burning of carbon. According to the equation (1):

$$m_{SnS_2} = {}^{\Delta m}/_{M_{SnO_2}} \times M_{SnS_2} \times 100\% \qquad (1)$$

Where n, M, Δm and m_{SnS2} are the quantity of matter, molar mass, the content of SnO_2 and , SnS_2 respectively.

The contents of SnS_2 and carbon are calculated to be 78.8% and 21.2%, respectively.

Table S1 The comparison of the electrochemical stability of C-SnS_2@rGO-0.2 with other with/without protective layer for SnS_x-based materials reported in previous literatures.

Samples	Current (A g^{-1})	Reversible Capacity (mAh g^{-1})	Cycle number	Ref.
C-SnS_2@rGO-0.2	**0.1**	**1428.7**	**300**	**This work**
	1.0	**938.4**	**400**	
	2.0	**704**	**1000**	
	5.0	**453**	**500**	
TC-RGO-CNT	0.5	100	150	[52]
SnS@G	0.1	1462	200	[48]
	1.0	1020	500	
MXene-decorated SnS_2 /Sn_3S_4	0.1	462.3	100	[53]
	5.0	101.4	500	
graphene@SnS_2	0.3	664	200	[54]
SnS_2/MoS_2/CFC	0.1	1294	120	[55]
SnS_2/CN	0.1	444.7	100	[56]
SnS_2/rGO/SnS_2	0.1	1357	200	[30]
	1.0	909	200	
SnS_2/rGO	0.1	1010	200	[57]
	1.0	910	1000	
SnS@SG	0.1	800	100	[49]
	1.0	527	300	
SnS_2	0.1	912	100	[50]
	0.5	800	300	
SnS_2@C	0.1	1150	200	[58]

	1.0	676	500	
rGO/SnS_2/TiO_2	1.0	485	200	[59]
SnS/MoS_2–C	0.2	989.7	60	[60]
	2.0	718	700	
SnS_2@C	0.1	690	100	[51]
	1.0	435	150	