Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting Information

Electronic Structure and Chemical Bonding of Graphene Oxide-Sulfur Nanocompoiste for Use in Superior Performance Lithium/Sulfur Cells

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I. NEXAFS spectra fitting procedure

The NEXAFS spectra at the C and O K edges were recorded in the total electron yield mode. The resolution was set to 0.1 and 0.2 eV for C and O, respectively. The spectra were first normalized by the incident beam intensity measured concomitantly using the photoelectron yield of a clean gold grid located upstream from the analysis chamber, and then normalized to the absorption pre- and post-edges. For the peak-fittings, the NEXAFS spectrum was first subtracted an arctan function background. It should be mentioned that the position of inflection point in the arctan function can strongly affect the areas of fitted peaks in each spectrum. However, the inflection point is usually obscured and it is difficult and complicated to determine it accurately.[1,2] Since we only care about the peak position of each component in the spectrum, the position of the inflection point will not have influence on our final results. For convenience, we have set the inflection point at ~286.5 and ~535.0 eV for C and O, respectively.[1,2] After subtracting the background, the spectrum was fitted with several Gaussian functions to get minimal residuals. The intensity of a Gaussian function is represented by[1]

$$I_G = H_G \exp\left[-\frac{1}{2}\left(\frac{E - P_G}{\frac{W_G}{c}}\right)\right] \qquad (1)$$

Where H_G is the maximum value of the Gaussian function; W_G is the full width at half maximum of the peak; P_G is the position of the peak; E is the independent variable in eV and $c = 2(\ln 4)^{1/2}$.

II. Conductivity of the prepared materials

Table 1. Conductivities of the prepared materials.

Sample name	GO	Heat treated GO[a]	Heat treated GO-S nanocomposites[a]
Conductivity (S cm^{-1})	0.00129	0.316	0.105

[a] These materials were heat treated in Ar environment at 155°C for 720 min.

III. Li/S cells assembly

The GO-S nanocomposite was mixed with carbon black and polyvinylidene difluoride (PVDF) with a weight ratio of 70:20:10 in N-Methylpyrrolidone (NMP) solvent to form a slurry. The slurry was uniformly spread using doctor blade onto a clean aluminum foil and then dried at 50 ℃ for 72 hours to form the working electrode. The final S content of the cathode material is about 46.2 %.

CR2032 type coin cells were assembled by using the as-prepared working electrode and Li metal foil (Cyprus Foote Mineral, 99.98 %, USA) as the counter electrode inside a high purity argon-filled glove box. The electrolyte was 1.0M/kg Lithium bis(trifluoromethane sulfonyl)imide (LiTFSI, 99.95 %, Aldrich) in N-methy-N-butylpyrrolidinium bis(trifluoromethanesulfonyl)imide ($PYR_{14}TFSI$, ~98.0%, Aldrich) and poly(ethylene glycol) dimethy ether (PEGDME, Mw = 250, Aldrich) (weight ratio 1:1).

IV. Electrochemical measurement

Galvanostatic discharge and charge measurements were made using an Arbin automatic battery cycler (BT-2000) between cut-off potentials of 1.0 and 3.0 V at room temperature. The capacity values were calculated according to mass of S in the cathode electrode.

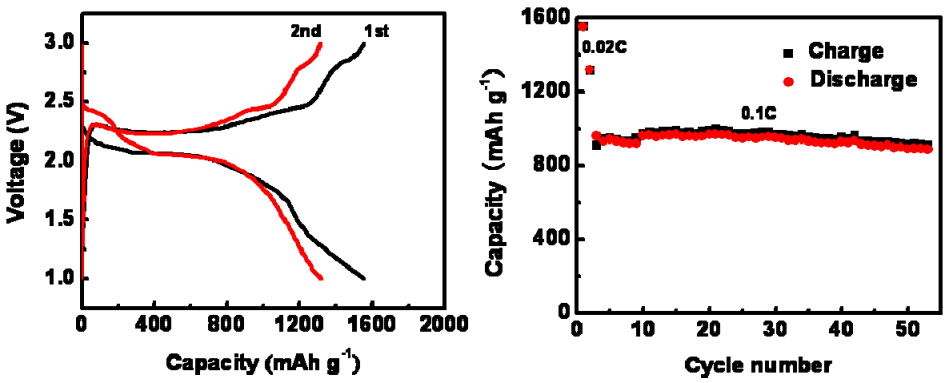

Figure S1. (a) Galvanostatic discharge/charge profiles of GO-S nanocomposite at 0.02C rate; (b) cycling performance of GO-S nanocomposite at a constant current rate of 0.1C after initial activation processes at 0.02C for two cycles.

References

(S1) Outka, D. A.; Stohr, J. *J. Chem. Phys.* **1988**, *88*, 3539.

(S2) Klein, R. J.; Fischer, D. A.; Lenhart, J. L. *Langmuir* **2011**, *27*, 12423.