Supporting Information

Understanding the function of cetyltrimethyl ammonium bromide in Lithium/Sulfur Cells

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Contents

Abbreviations used in this Supporting Information

S-GO-CTA: composite of sulfur, graphene oxide and cetyltrimetylammonium bromide (CTAB), TGA: Thermogravimetric analysis, Me_2S_x: Dimethyl polysulfide, CA: cetylamine, CMA: etylmethylamine, CDMA: cetyldimethylamine, MS: mass spectrometry, S-CTA: model composite of sulfur and CTAB, NMR: nuclear magnetic resonance spectrometry, H_2S_x: Hydrogen polysulfides, XRD: X-ray diffraction, S-CDMA: model composite of sulfur and CDMA.

Fig. S1 Graphical explanation of the method to calculate the contents in S-GO-CTA.

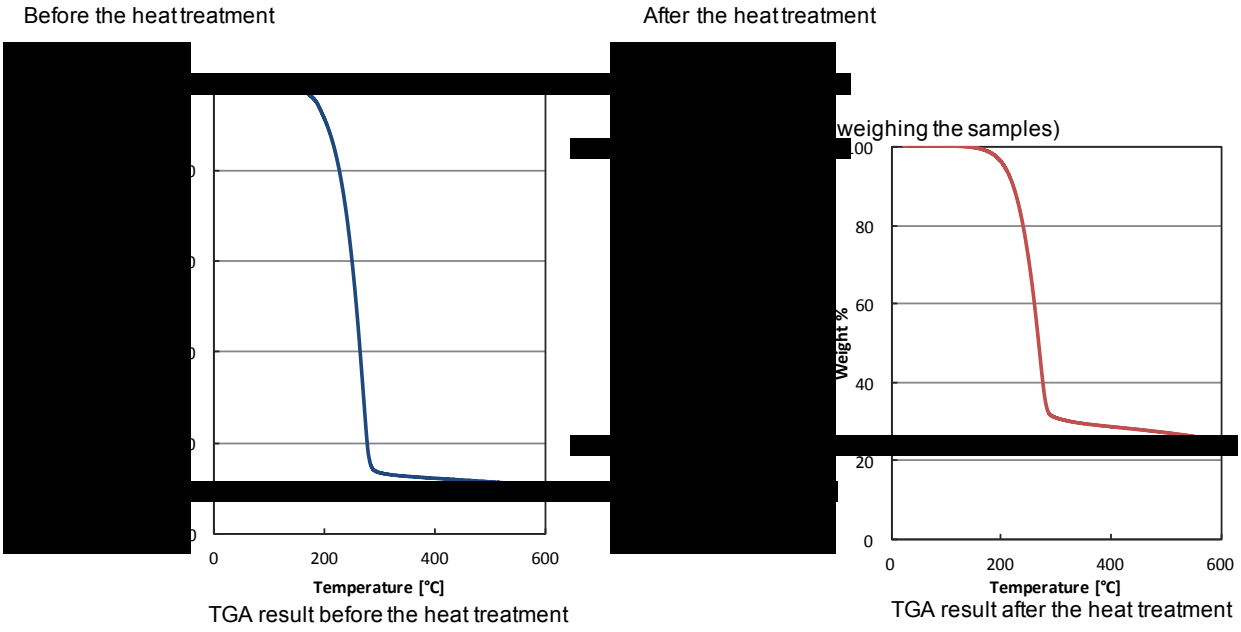

Fig. S1 Graphical explanation of the method to calculate the contents of sulfur and Phase X produced during the heat treatment in S-GO-CTA using the TGA results and the measurement of the weight of the samples before and after the heat treatment.

Fig. S2 TGA results of references.

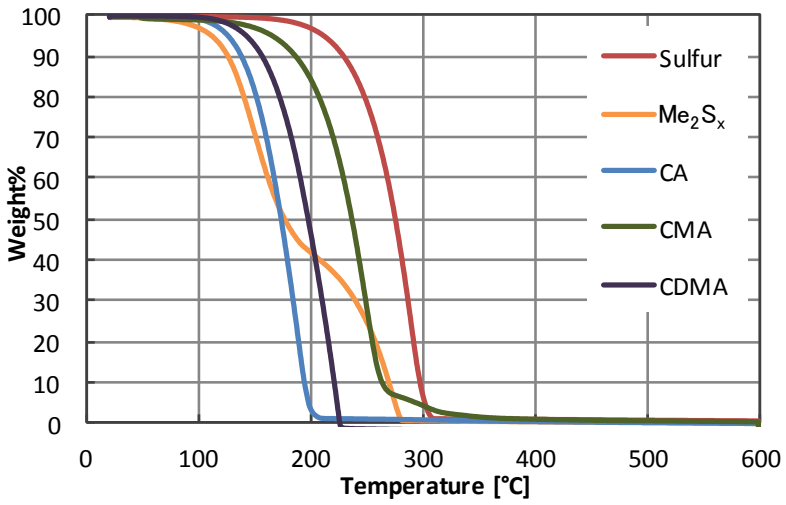

Fig. S2 TGA results of sulfur, Me_2S_x, CA, CMA and CDMA as references.

Fig. S3 MS spectrum of S-CTA model compound with the theoretical isotope pattern.

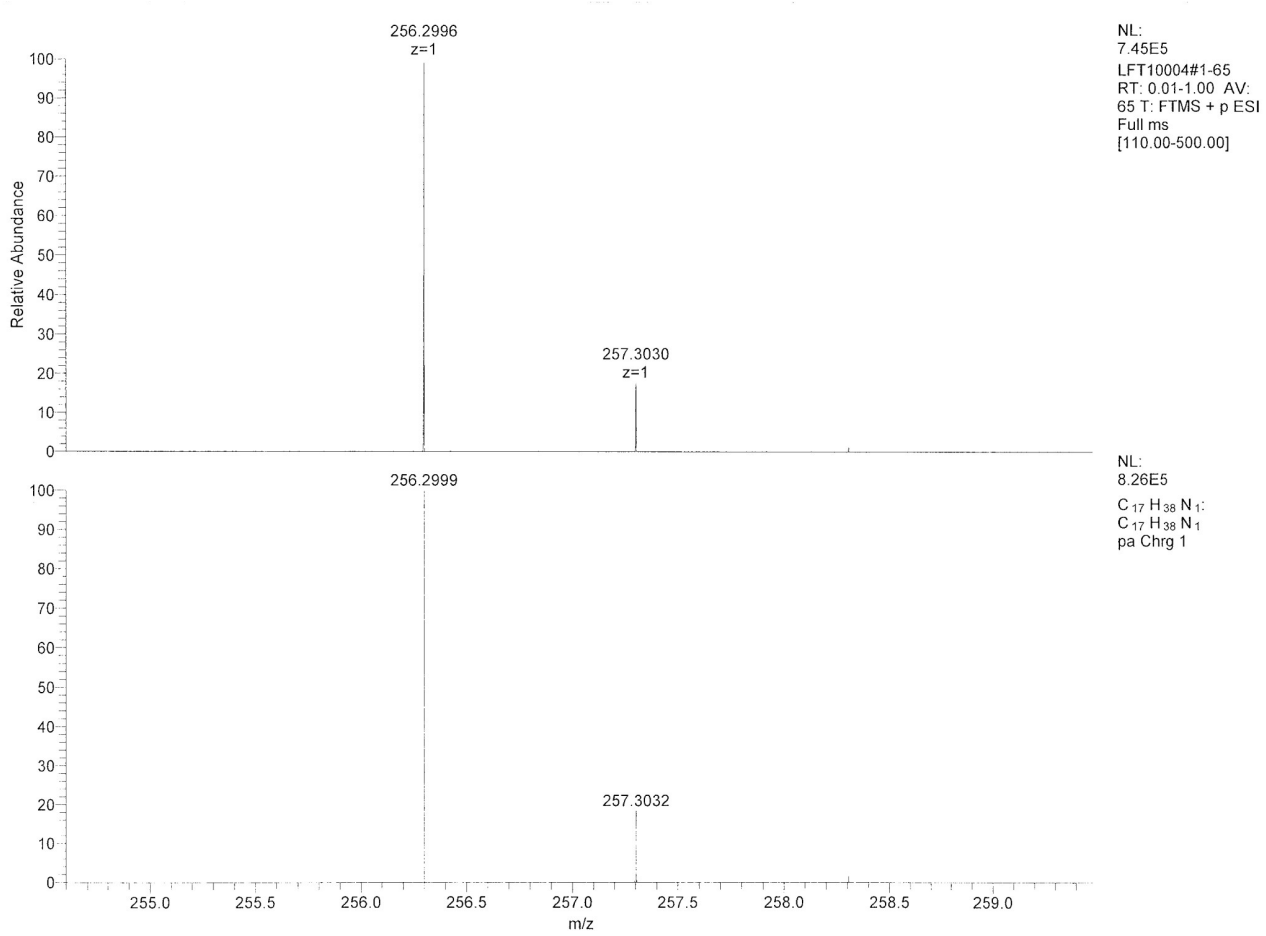

Fig. S3 ESI-MS spectrum of S-CTA model composite after the heat treatment with the theoretical isotope pattern to identify CMA.

Fig. S4 1H NMR spectra of S-GO-CTA composite.

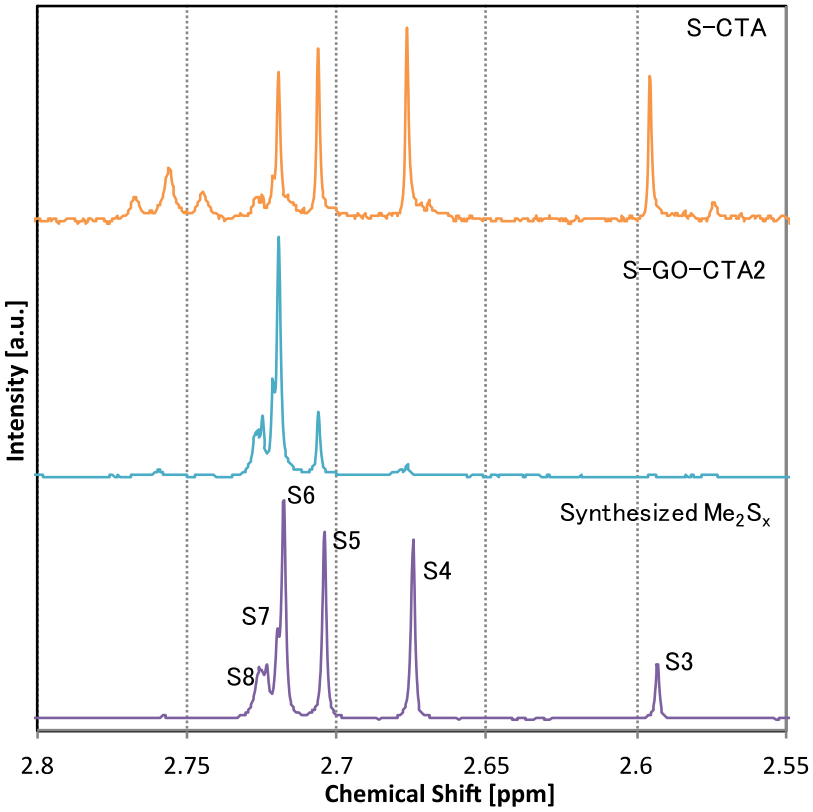

Fig. S4 Enlarged NMR spectra of S-CTA, S-GO-CTA2 and Me_2S_x as reference to identify Me_2S_x produced in S-CTA and S-GO-CTA after the heat treatment.

Fig. S5. 13C NMR spectra of S-GO-CTA composite.

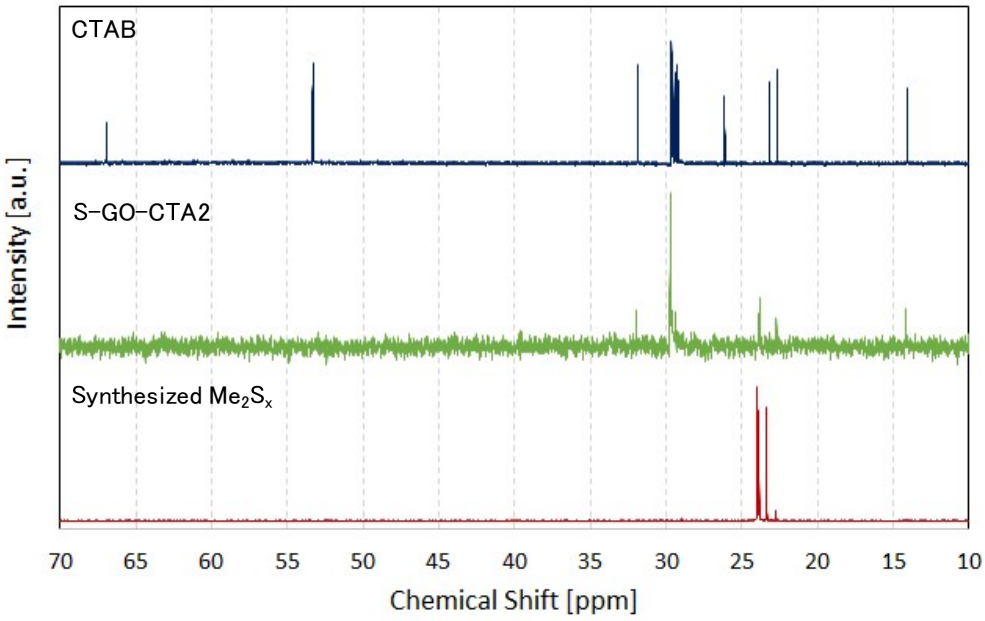

Fig. S5 13C NMR spectrum of S-GO-CTA after the heat treatment, and the spectra of CTAB and Me_2S_x as references.

Fig. S6 1H NMR spectra of S-GO-CTA composite.

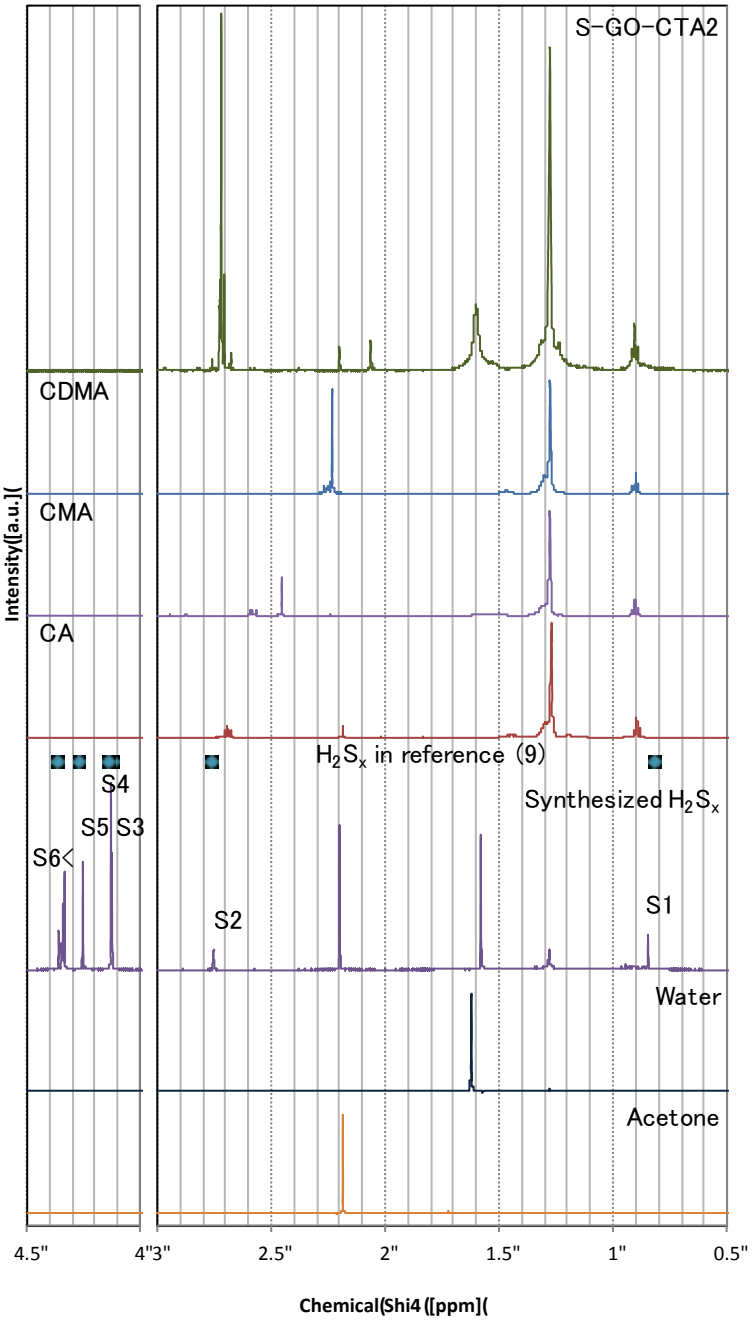

Fig. S6 1H NMR spectra of S-GO-CTA2 with reference spectra of synthesized H_2S_x, water, acetone and three types of amines, CDMA, CMA and CA.

Fig. S7 XRD patterns of S-GO composite.

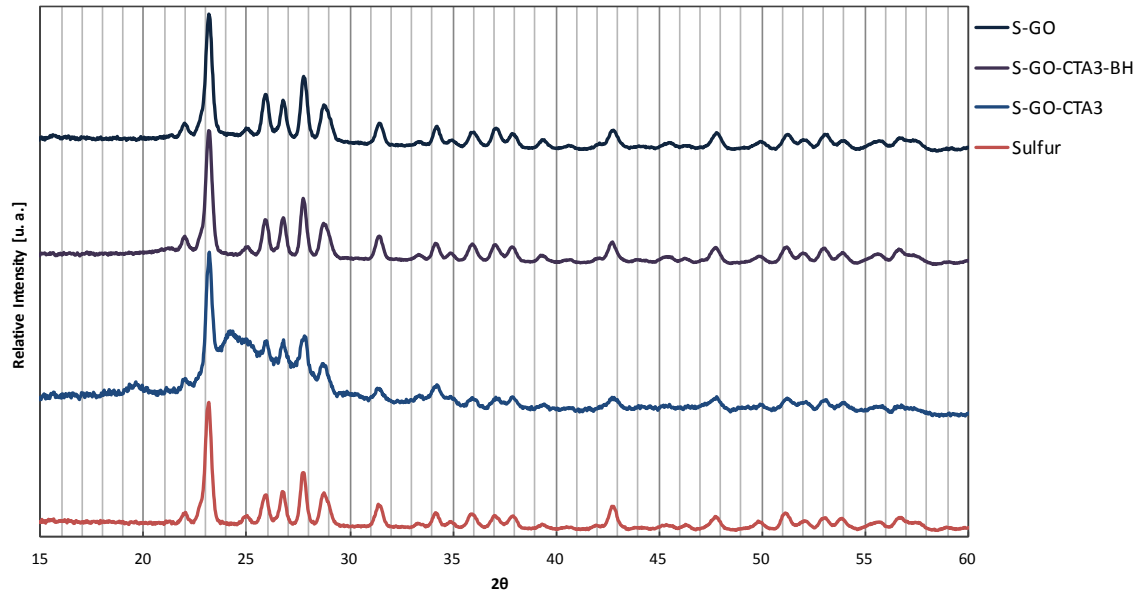

Fig. S7 XRD patterns of S-GO-CTA with and without CTAB and before and after the heat treatment with reference of sulfur.

Fig. S8 MS spectra of S-CDMA model compound with the theoretical isotope pattern.

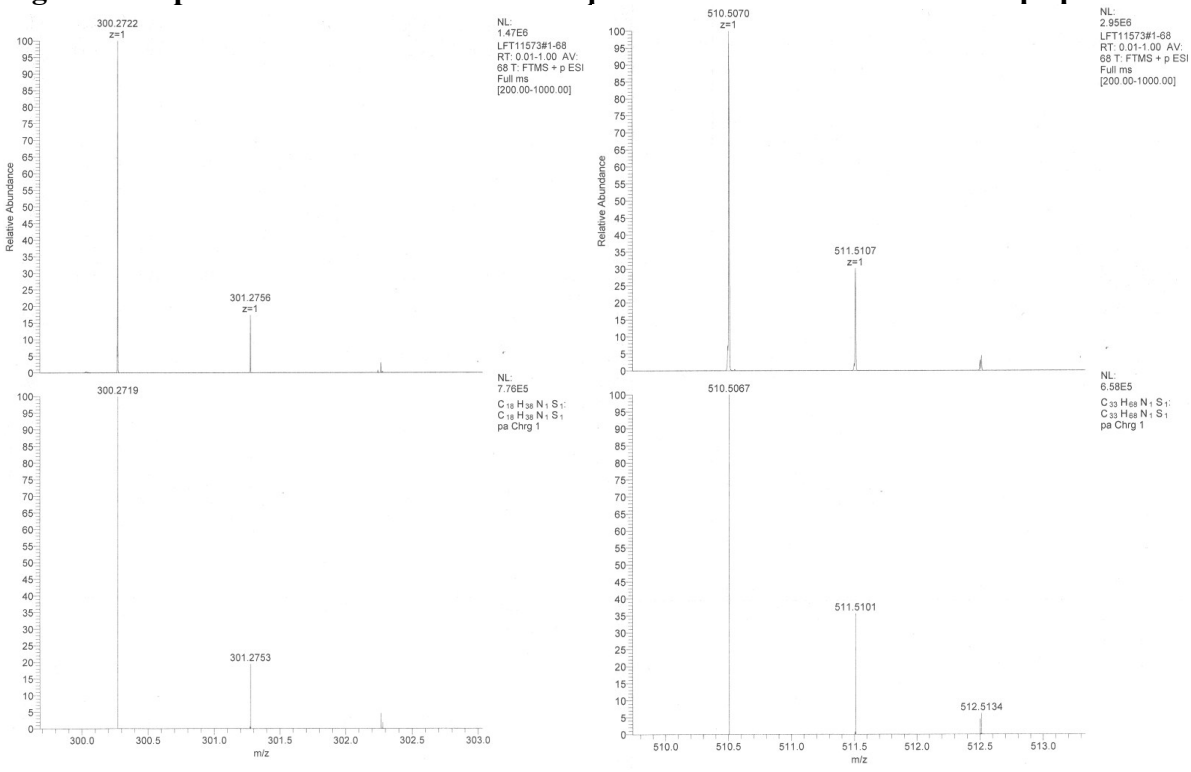

Fig. S8 MS spectra of S-CDMA model composite after the heat treatment with the theoretical isotope pattern corresponding to the part to identify (a) Cetylmethylaminomethanethiol (S-CDMA-1) and (b) N-cethyl-1-cetylsulfanylmethanamine (S-CDMA-2).

Fig. S9 XAS spectra of S-GO composite.

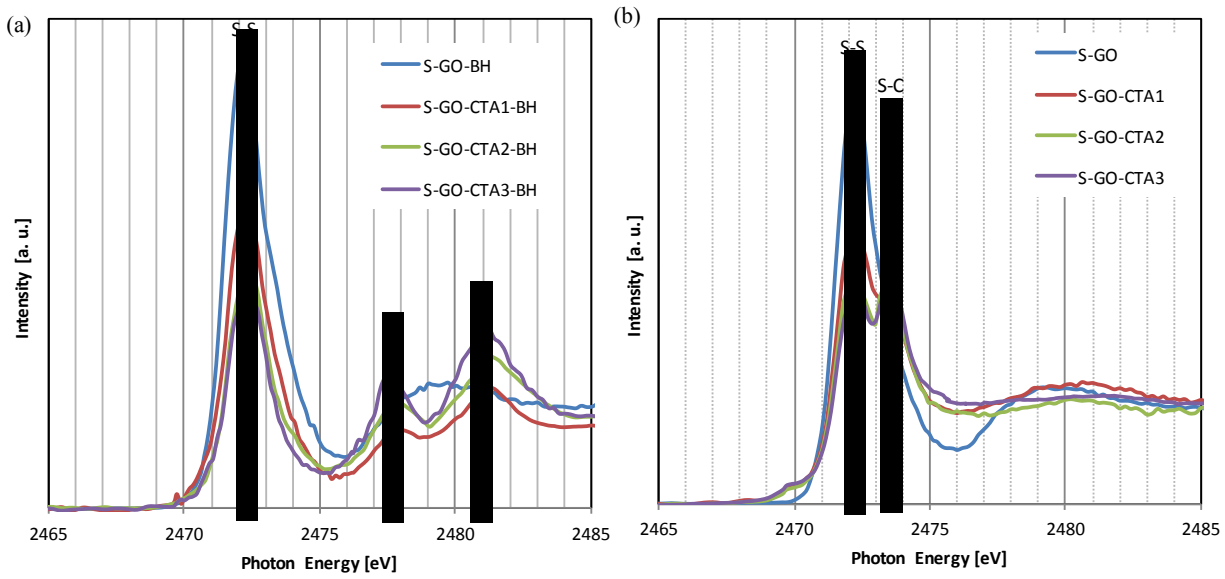

Fig. S9 XAS spectra of S-GO-CTA composite having different amount of CTAB before the heat treatment (a) and after the heat treatment (b).

Fig. S10 Raman spectra of references.

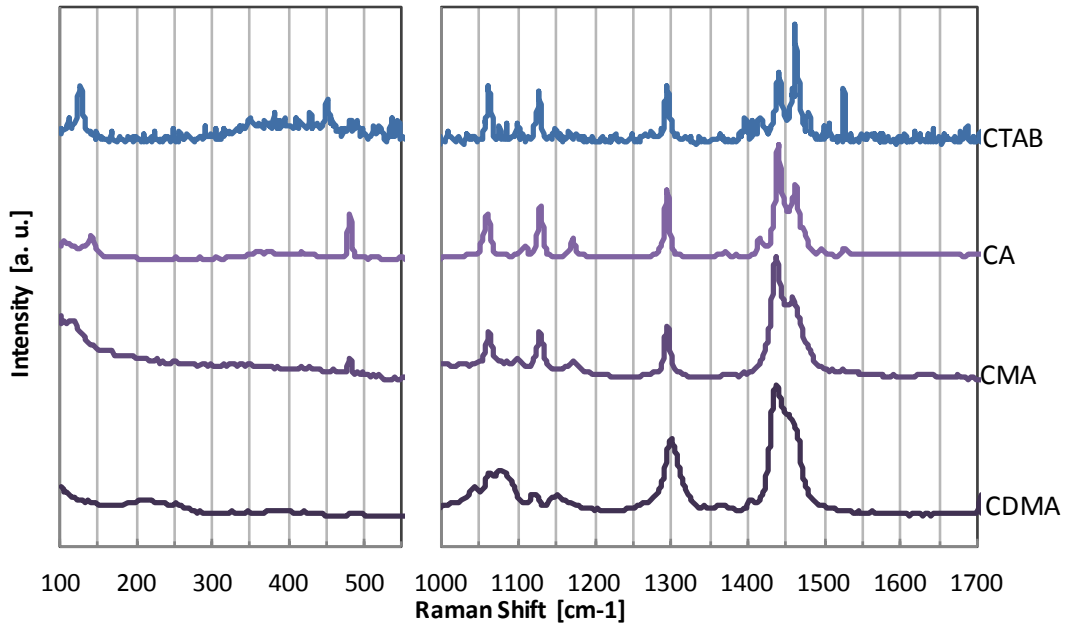

Fig. S10 Raman spectra of CTAB, CA, CMA and CDMA as references.

Fig. S11 Theoretically calculated Raman spectra of amine compounds.

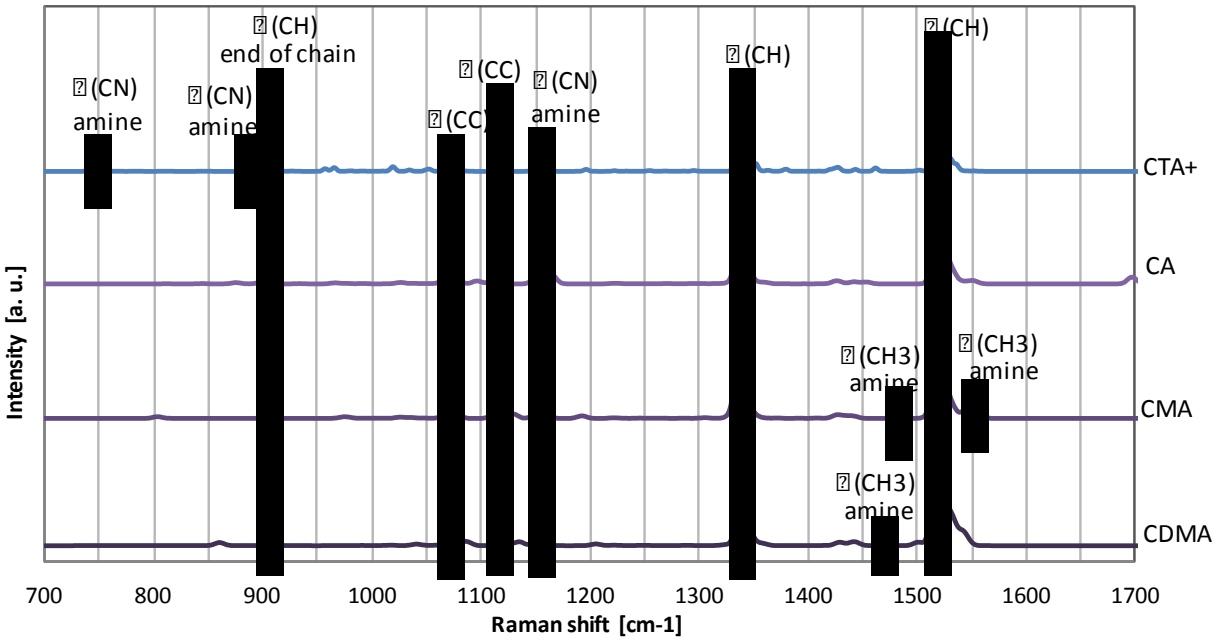

Fig. S11 Theoretically calculated Raman spectra of CTA^+, CA, CMA and CDMA with their vibration modes by using optimized models.

Fig. S12 SEM images of S-GO-CTA composite.

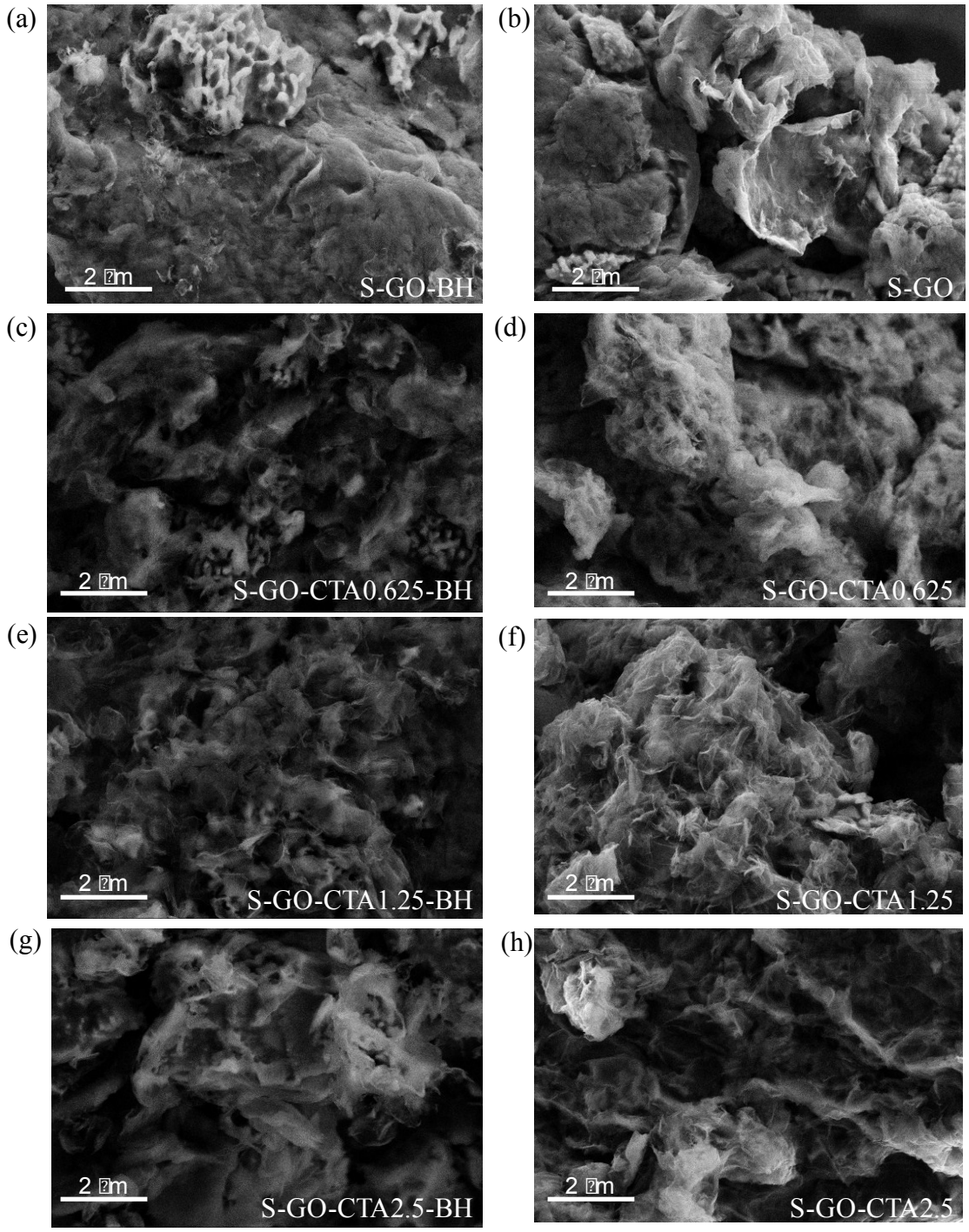

Fig. S12 SEM images of S-GO-CTA composites having different amount of CTAB before and after the heat treatment.

Fig. S13 Cyclic voltammetry of S-GO-CTA composites.

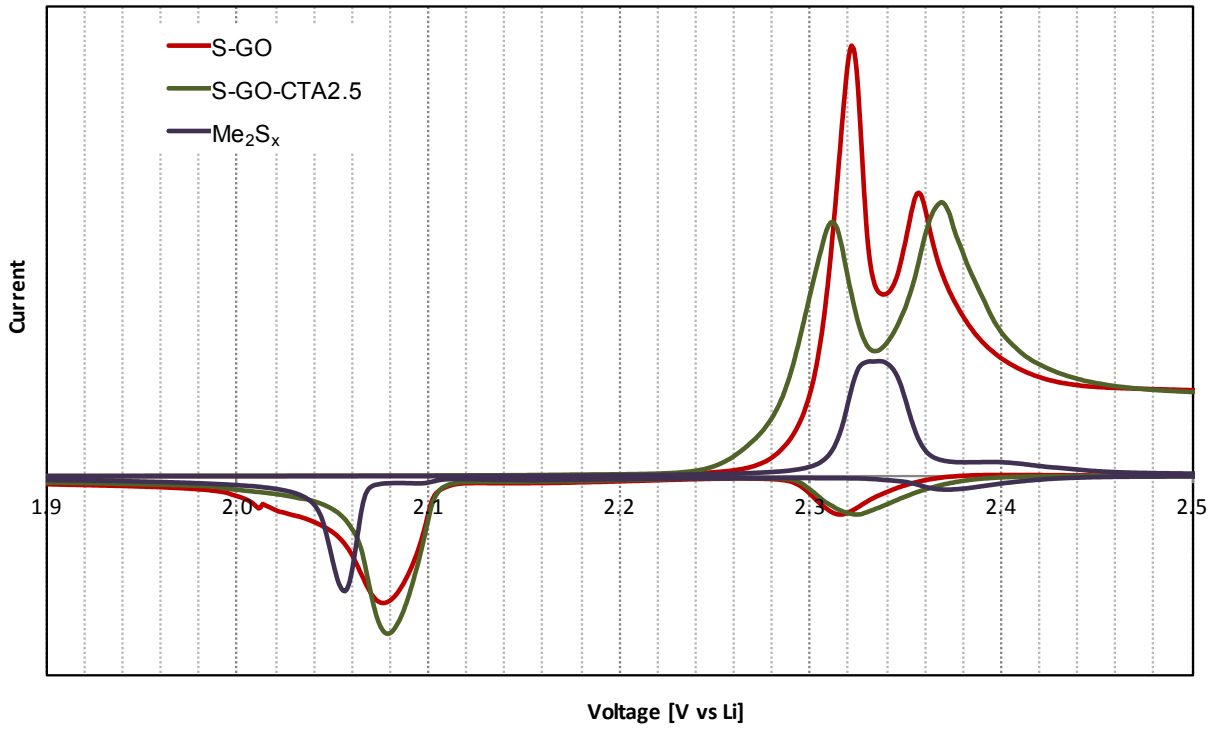

Fig. S13 Cyclic voltammetry of S-GO-CTA composites having CTAB and no CTAB and dimethylpolysulfide.

Fig. S14 Voltage profiles of S-GO-CTA composites.

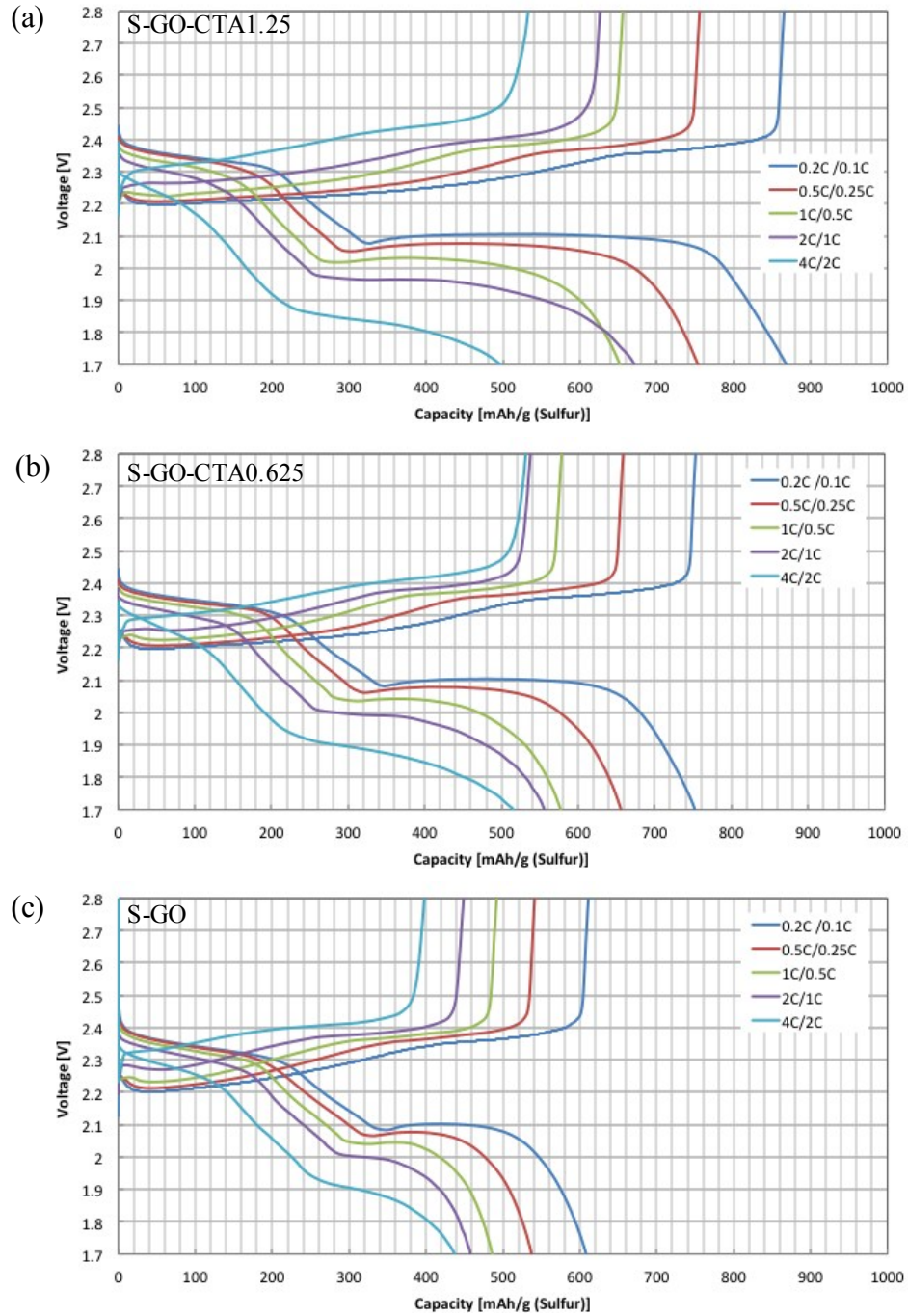

Fig. S14 Voltage profiles of (a) S-GO-CTA1.25, (b) S-GO-CTA0.625 and (c) S-GO at different C rates. C rate in discharge and charge are indicated on left side and right side of the slash respectively.

Fig. S15 Voltage profiles of S-GO-CTA composites for the first 5 cycles.

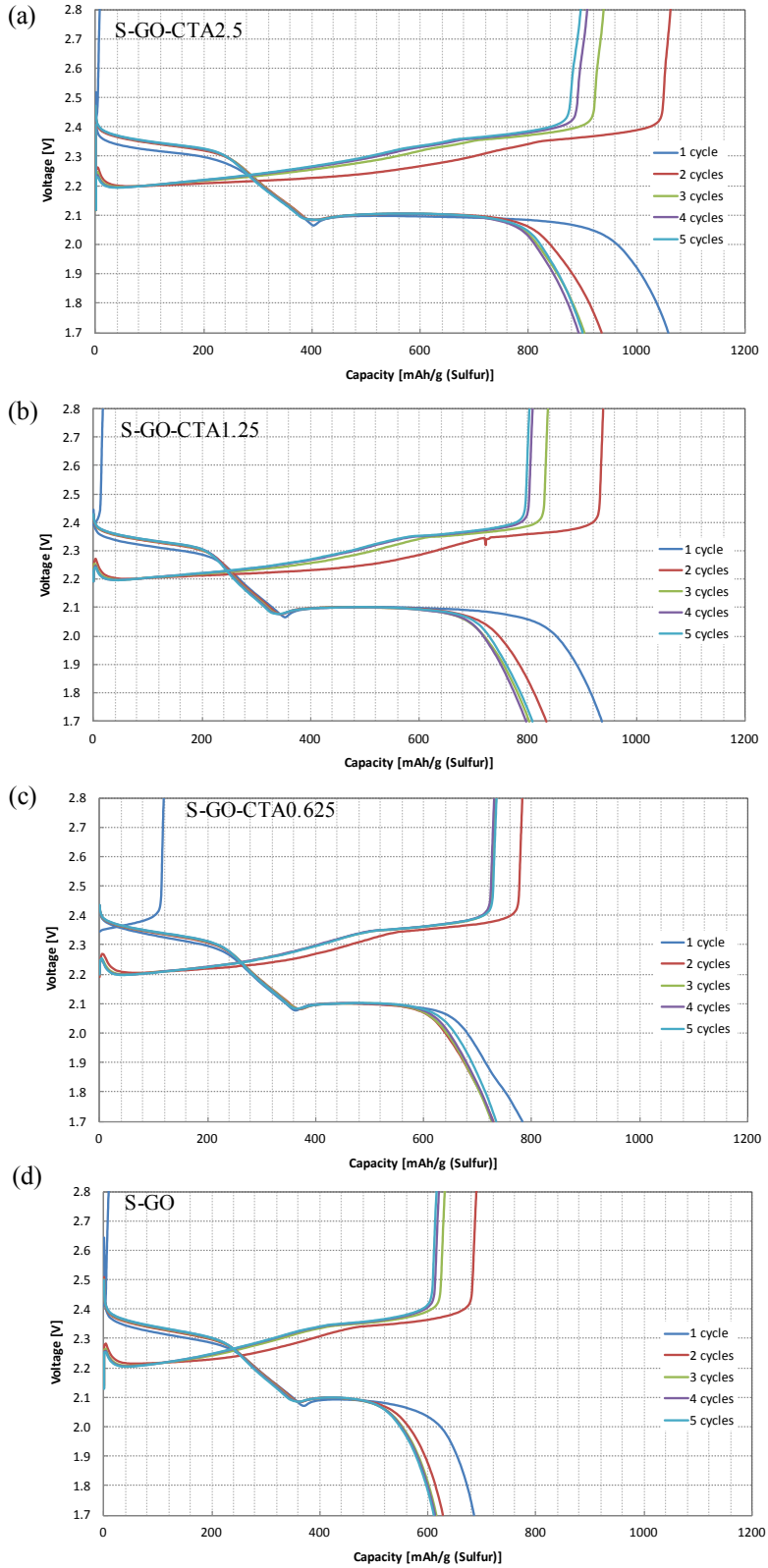

Fig. S15 Voltage profiles of (a) S-GO-CTA2.5, (b) S-GO-CTA1.25, (c) S-GO-CTA0.625 and (d) S-GO for the first 5 cycles.

Fig. S16 Voltage profiles of S-GO-CTA composites after 100 cycles.

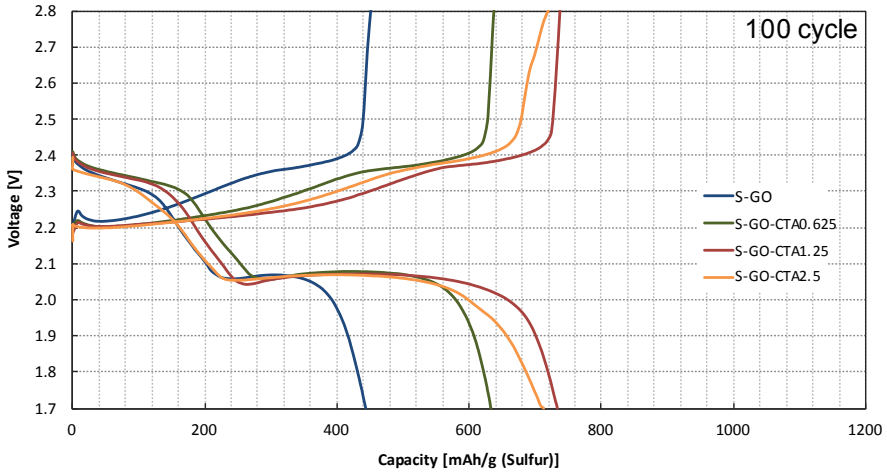

Fig. S16 Voltage profiles of S-GO-CTA2.5, S-GO-CTA1.25, S-GO-CTA0.625 and S-GO after 100 cycles.