

Supporting Information

Short-Chain Polyselenosulfide Copolymers as Cathode Materials for Lithium-Sulfur Batteries

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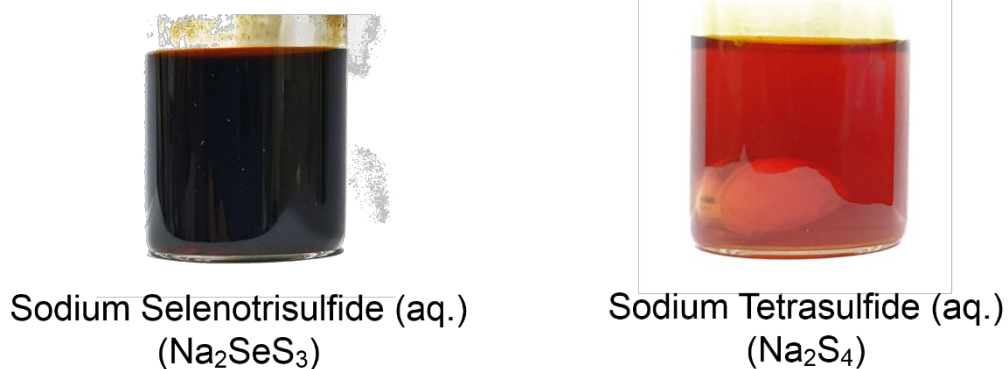


Figure S1. Digital photographs of 1 M aqueous sodium selenotrisulfide (Na_2SeS_3) and 1 M sodium tetrasulfide (Na_2S_4) precursor solution

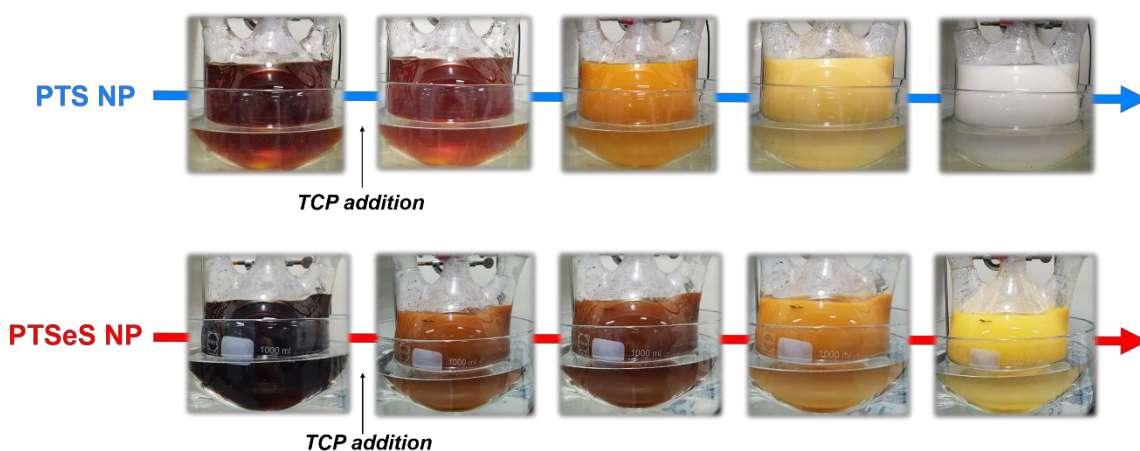
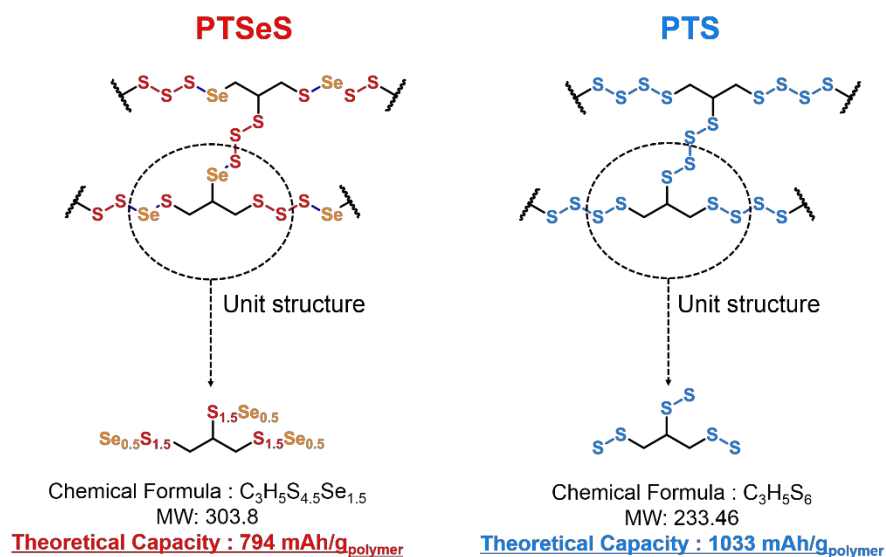


Figure S2. Visual changes of reaction medium during polymerization. Upon addition of 1,2,3-trichloropropane (TCP), $\text{S}_{\text{N}}2$ -based polycondensation reaction took place between nucleophilic sodium polyselenosulfides ($\text{Na}_2\text{Se}_x\text{S}_{4-x}$, ($x=1$ or 0)) and electrophilic C-Cl units of TCP. Final products were obtained as aqueous dispersion of polymer nanoparticles (size~200 nm) which resulted in opaque suspension. We should note that as PTSeS and PTS are insoluble in most of organic solvents due to their highly cross-linked nature, solution based characterization techniques (e.g. gel permeation chromatography (GPC) for measuring molecular weight) were not applicable.



- **C-S** (or **C-Se**): Take up 1 equivalent of Li^+ and e^- to form **C-SLi** (or **C-SeLi**)
- **-S-** (or **-Se-**) in the middle of chain : Take up 2 equivalent of Li^+ and e^- to form **Li₂S** (or **Li₂Se**)

∴ For the unit structure of both polymer, $3*2 + 3*1 = 9$ electrons are involved in redox reaction

Theoretical Capacity = $96485 * 9 / MW(\text{unit structure}) / 3600$ [mAh/g_{polymer}]

Figure S3. Calculation of theoretical specific capacity of PTSeS and PTS

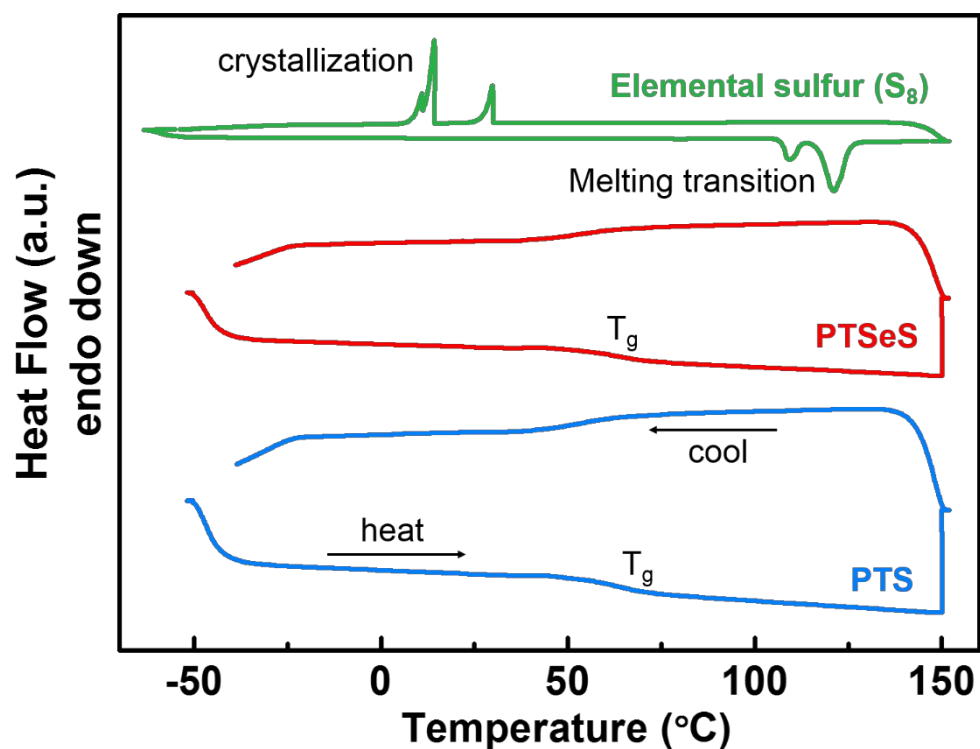


Figure S4. Differential scanning calorimetry (DSC) thermograms of PTSeS, PTS and sulfur

Table S1. Elemental analysis (EA) results and theoretical elemental composition of PTSeS and PTS

	PTS NP		PTSeS NP	
	Experimental	Theoretical	Experimental	Theoretical
C	15.78 (21.64)	15.43	9.36 (18.69)	11.86
H	2.20 (35.87)	2.16	1.35 (32.11)	1.66
S	82.73 (42.49)	82.41	49.65 (37.15)	47.50
Se			*39.64 (12.04)	38.99

Unit: wt% (mol%)

*Calculated from $f_{\text{Se}} = 100 - (f_{\text{C}} + f_{\text{H}} + f_{\text{S}})$

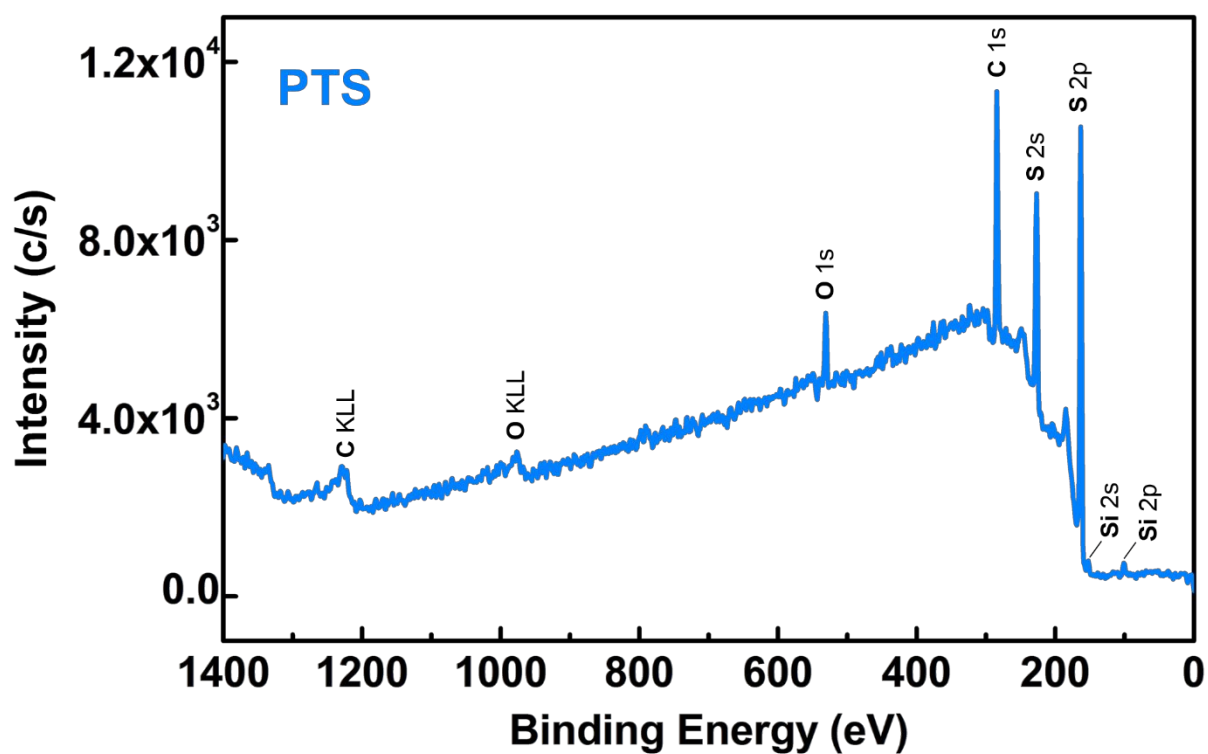
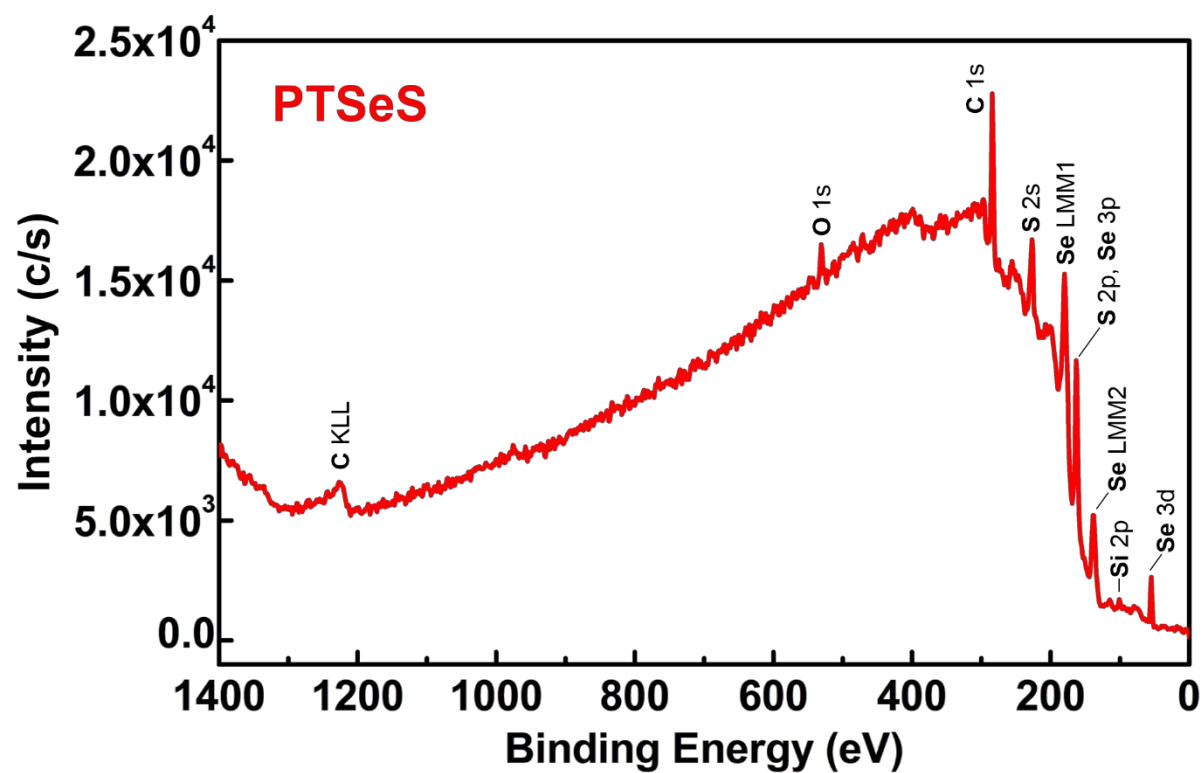


Figure S5. X-ray Photoelectron Spectroscopy (XPS) survey scanning spectra of PTSeS and PTS

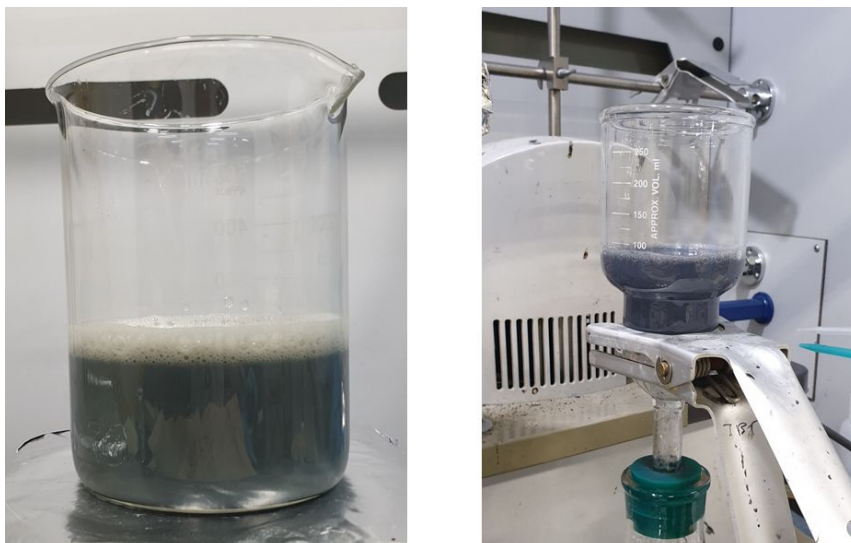


Figure S6. Digital photograph of homogeneous dispersion of PTSeS (75%), CG (18.75%) and CNT (6.25%) after ultra-sonication (left) and following vacuum-filtration to collect the PTSeS/CG-CNT composite (right).

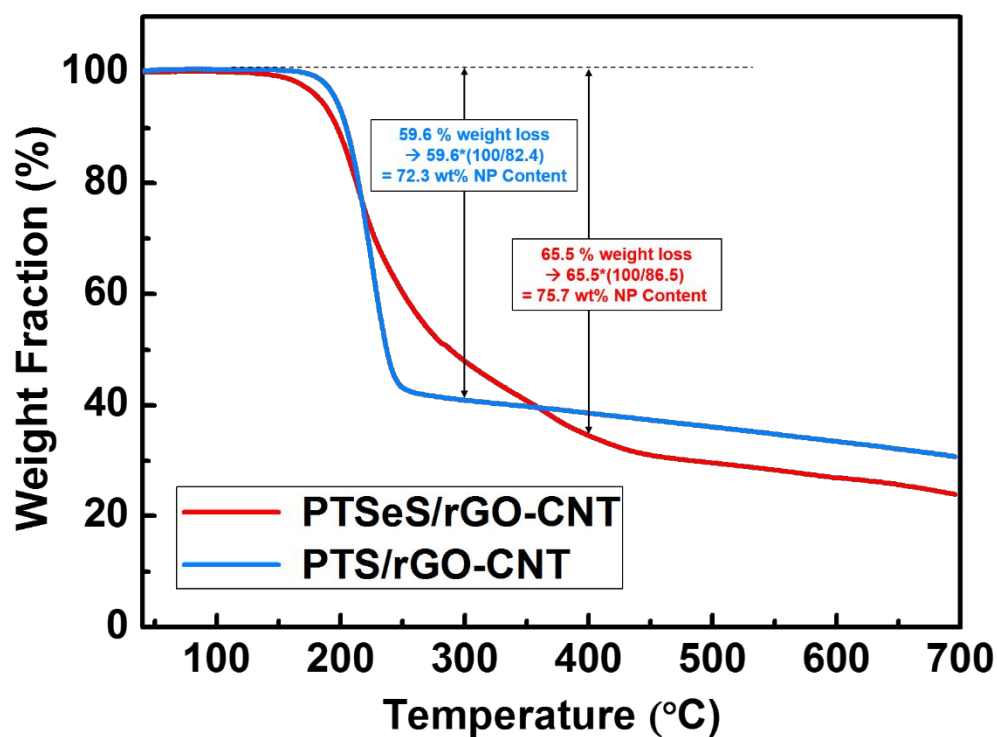


Figure S7. TGA curves of Polymer/rGO-CNT nanocomposites under N_2 atmosphere

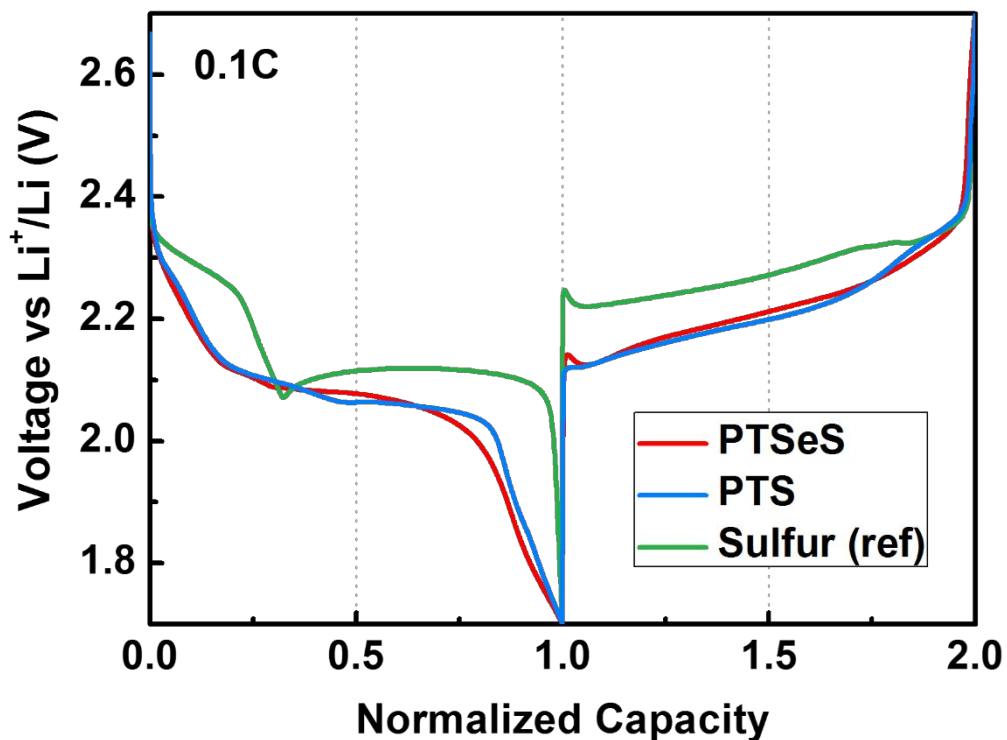


Figure S8. Normalized galvanostatic charge/discharge voltage profiles of PTSeS, PTS and sulfur

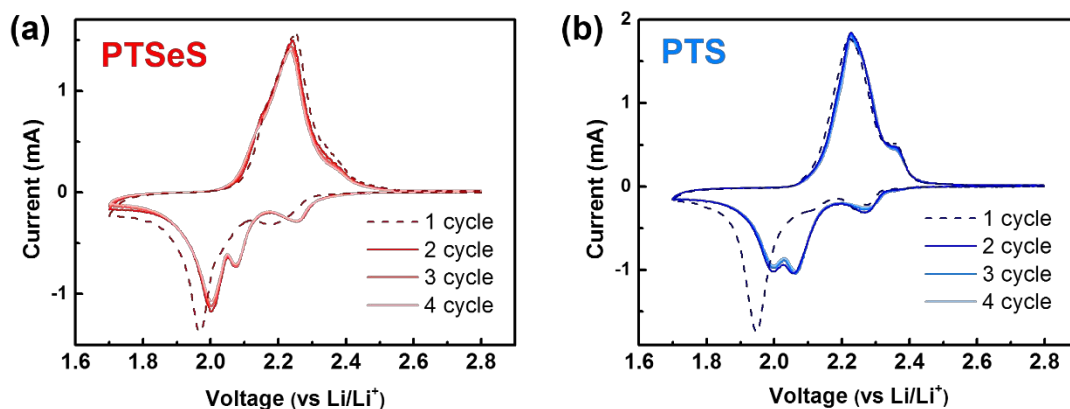


Figure S9. CV plots at 0.1 mV s^{-1} scan rate up to 4th cycle for (a) PTSeS and (b) PTS. 1st cycle of both polymers exhibited higher polarization than the subsequent cycles due to the spherical morphology of the NPs. After 1 cycle, the polymers lost their initial morphology and were redistributed over carbon frameworks of the electrode film. Thus, closer and contact between the polymers and conductive carbon and overall polarization became relieved.

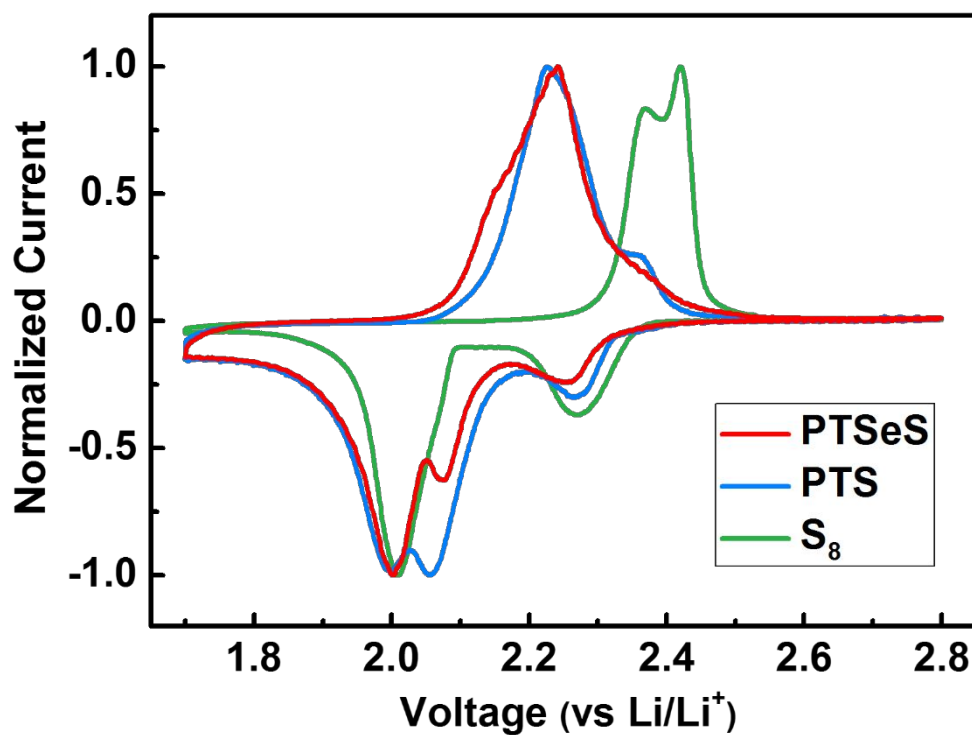


Figure S10. Normalized CV plots of PTSeS, PTS and sulfur

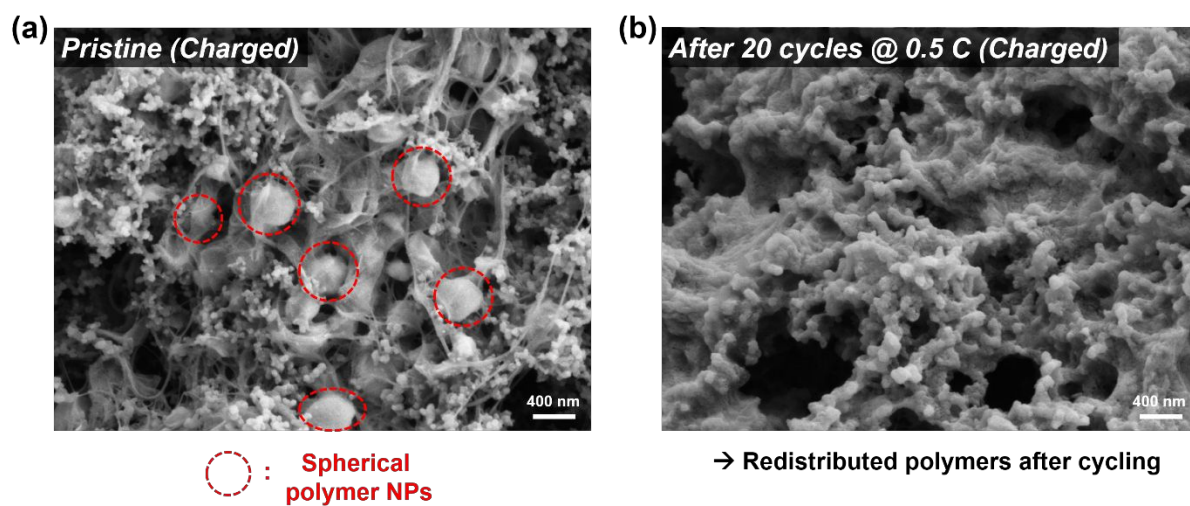


Figure S11. SEM images of the PTSeS/CG-CNT electrodes at (a) pristine charged state and (b) after 20 cycles (charged state) at 0.5 C current density

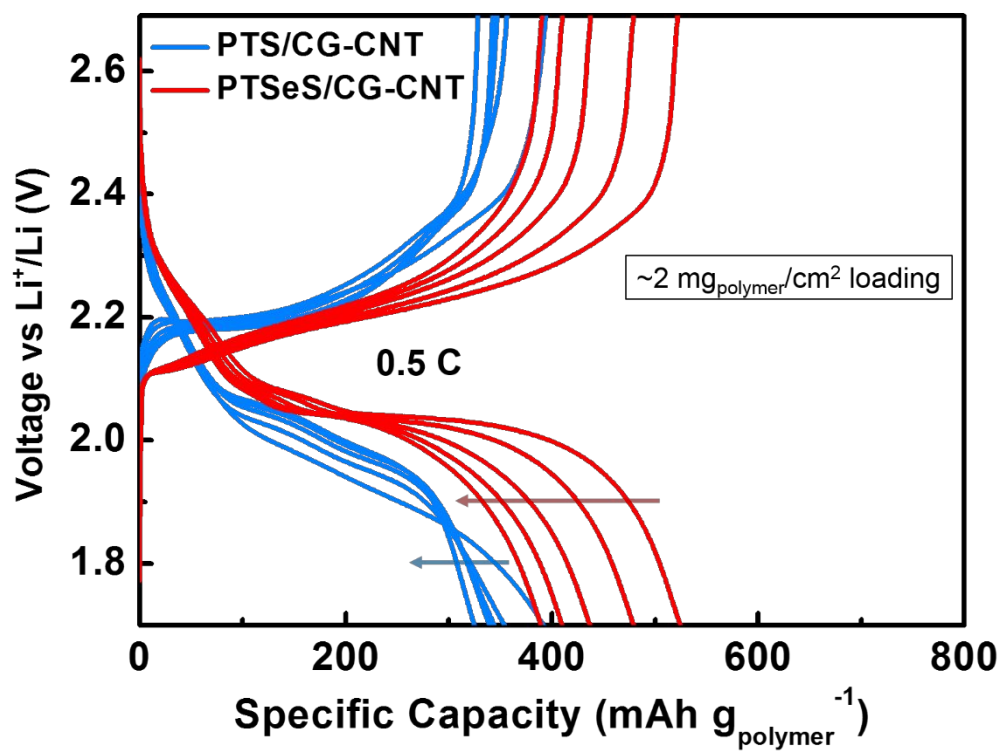


Figure S12. Charge/discharge voltage profiles of PTSeS/CG-CNT and PTS/CG-CNT cycled at 0.5 C with $\sim 2 \text{ mg}_{\text{polymer}} \text{ cm}^{-2}$ loading at 100, 200, 300, 400, 500th cycle

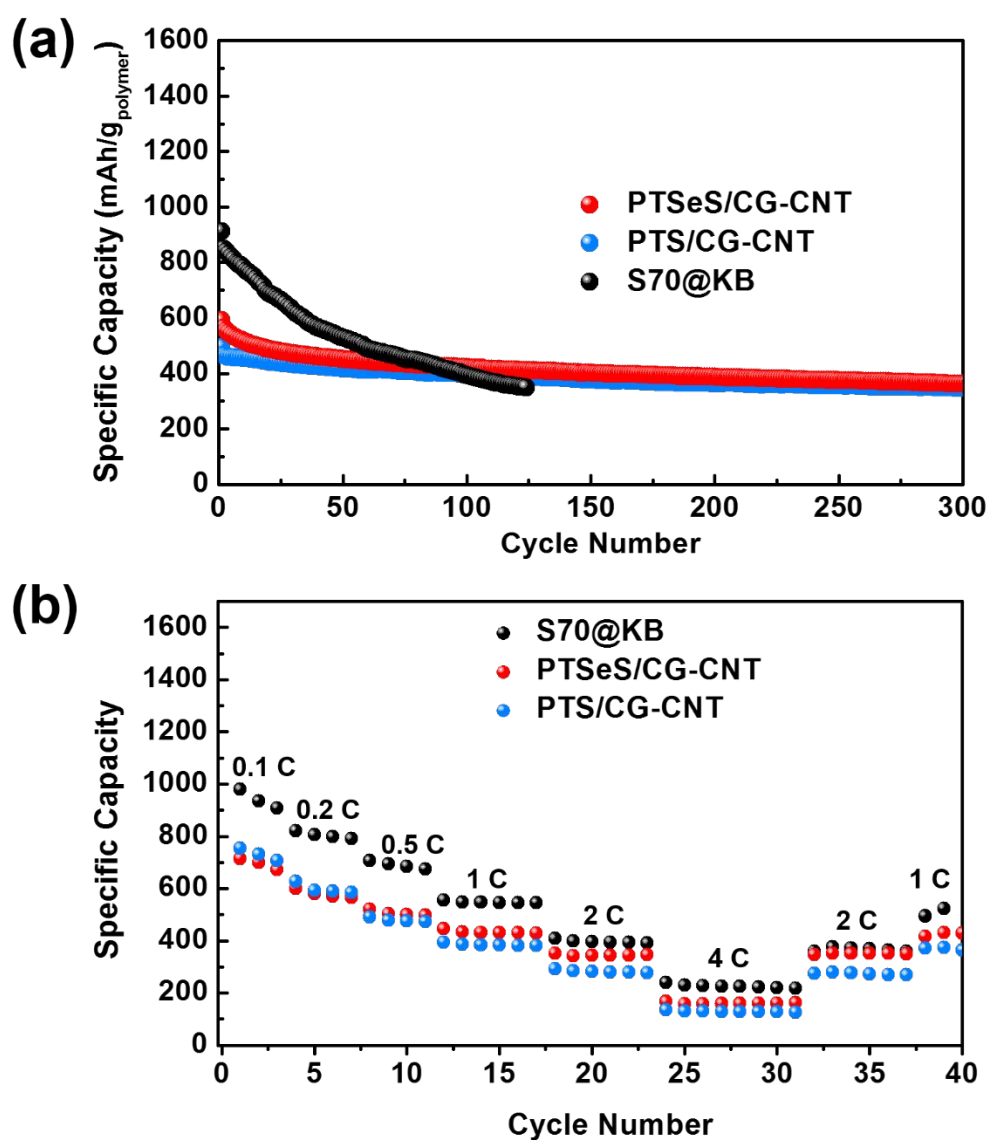


Figure S13. (a) Cycling performance and (b) rate capability of PTSeS/CG-CNT, PTS/CG-CNT ($\sim 1 \text{ mg}_{\text{polymer}}/\text{cm}^2$ loading) and typical S70@KB (70 wt% sulfur impregnated in to ketjen black) as reference electrode. S70@KB electrode was fabricated with 70:20:10 mass ratio of S70@KB:Super P:PVDF having same areal mass loading ($\sim 1 \text{ mg}$) of sulfur.

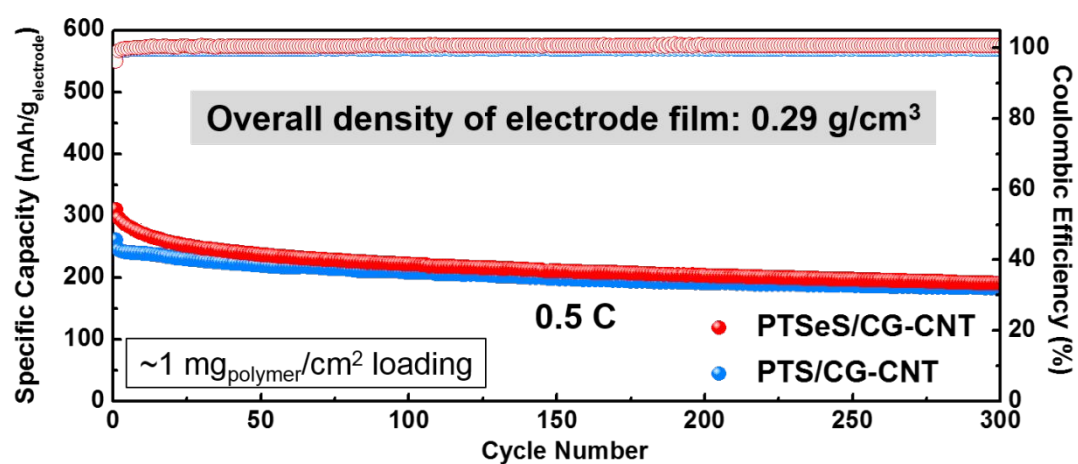


Figure S14. Cycling performance of PTSeS and PTS-based electrodes calculated based on the total mass of the electrode (active material+conductive agent+binder).