

Facile synthesis of BiSI and $\text{Bi}_{13}\text{S}_{18}\text{I}_2$ as stable electrode materials for supercapacitor applications

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Supporting information

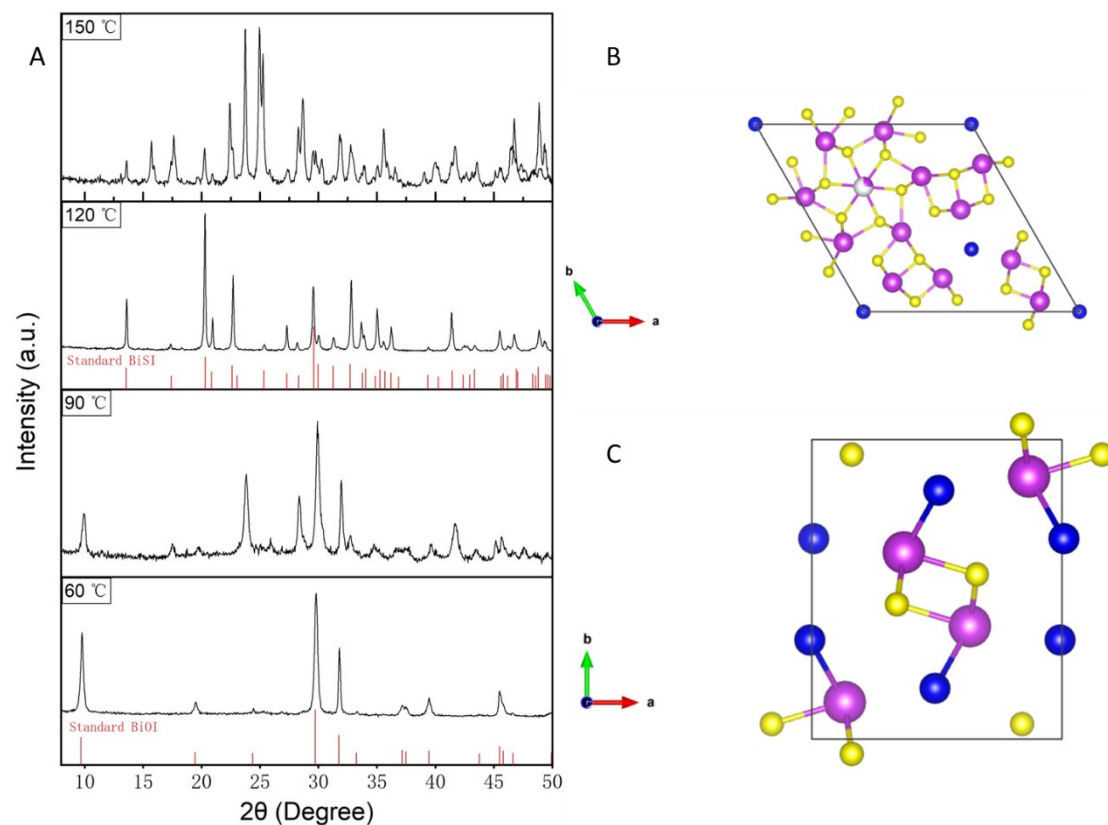


Figure S1. (A) XRD patterns of the as-prepared BiSI powder at different temperature, standard BiSI (ICDD PDF card No. 43-652) and standard BiOI (ICDD PDF card No. 10-0445). (B) Crystallographic packing diagram of $\text{Bi}_{13}\text{S}_{18}\text{I}_2$ unit cell. bismuth: magenta; iodine: blue; sulfur: yellow. The disordered bismuth is shown in grey with an occupancy factor of 0.25. (C) BiSI unit cell: bismuth: magenta; iodine: blue; sulfur: yellow.

Table S1. The experimental weight loss value and the theoretical weight loss value calculated from the three equations.

Steps	Theoretical weight loss (%) for BiSI	Observed weight loss (%) for BiSI	Theoretical weight loss (%) for $\text{Bi}_{13}\text{S}_{18}\text{I}_2$	Observed weight loss (%) for $\text{Bi}_{13}\text{S}_{18}\text{I}_2$
1	53.55	55.11		
2	47.61	44.61	88.91	87.86
3	34.60	37.48	72.68	73.91

Table S2. Atomic percentages of elements present in thin film as calculated from analysis of XPS compared with theoretical values in BiSI and $\text{Bi}_{13}\text{S}_{18}\text{I}_2$

Element /Orbital	At.% (BiSI-a)	Total	At. % in BiSI	At.% ($\text{Bi}_{13}\text{S}_{18}\text{I}_2$ -a)	Total	At. % in $\text{Bi}_{13}\text{S}_{18}\text{I}_2$
Bi / 4d 3	18.04			18.16		
Bi / 4d 5	15.82	33.86	33.33	20.36	38.52	39.39
I / 3d 3	18.09			3.81		
I / 3d 5	14.46	32.55	33.33	4.16	6.97	6.06
S / 2s	33.58	33.58	33.33	53.42	54.42	54.55

Table S3. Energy density and power density of (a) BiSI-a, (b) BiSI-b, (c) $\text{Bi}_{13}\text{S}_{18}\text{I}_2$ -a and (d) $\text{Bi}_{13}\text{S}_{18}\text{I}_2$ -b electrodes calculated from galvanostatic charge-discharge measurement.

(a)

Current density $\text{A} \cdot \text{g}^{-1}$	1	2	4	6	8	10
Energy Density Wh kg^{-1}	9.54	10.02	9.6	9.12	9	8.76
Power Density W kg^{-1}	240.5	626.2	1305.81	1435.3	1867	2494.3

(b)

Current density $\text{A} \cdot \text{g}^{-1}$	1	2	4	6	8	10
Energy Density Wh kg^{-1}	29.52	27.78	23.04	22.5	21.48	22.2
Power Density W kg^{-1}	251	648.2	1620.7	1765.2	2110.9	3150.2

(c)

Current density $\text{A} \cdot \text{g}^{-1}$	1	2	4	6	8	10
Energy Density Wh kg^{-1}	4.63	4.48	4.52	4.46	4.42	4.34
Power Density W kg^{-1}						

(d)

Current density $\text{A} \cdot \text{g}^{-1}$	1	2	4	6	8	10
Energy Density Wh kg^{-1}	3.71	3.62	3.6	3.32	3.28	3.15
Power Density W kg^{-1}	265	525.48	1098.3	1867.5	2270.8	2700

Table S4 controlled capacitance of carbon paper and additive

Current density $\text{A} \cdot \text{g}^{-1}$	1	2	4	6	10
Specific Capacitance Fg^{-1}	0.84	0.8	0.72	0.68	0.46

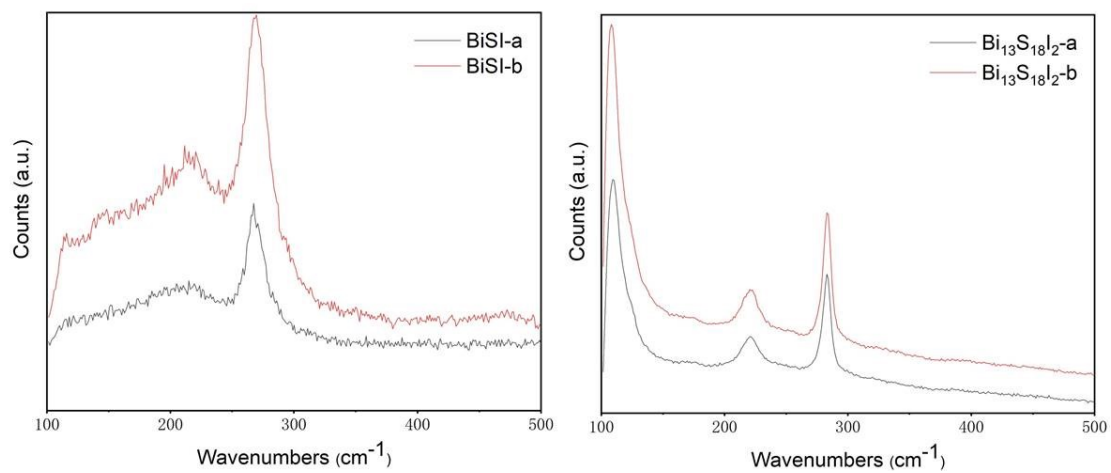


Figure S2. Raman spectra of BiSI-a, BiSI-b, Bi₁₃S₁₈I₂-a, and Bi₁₃S₁₈I₂-b.

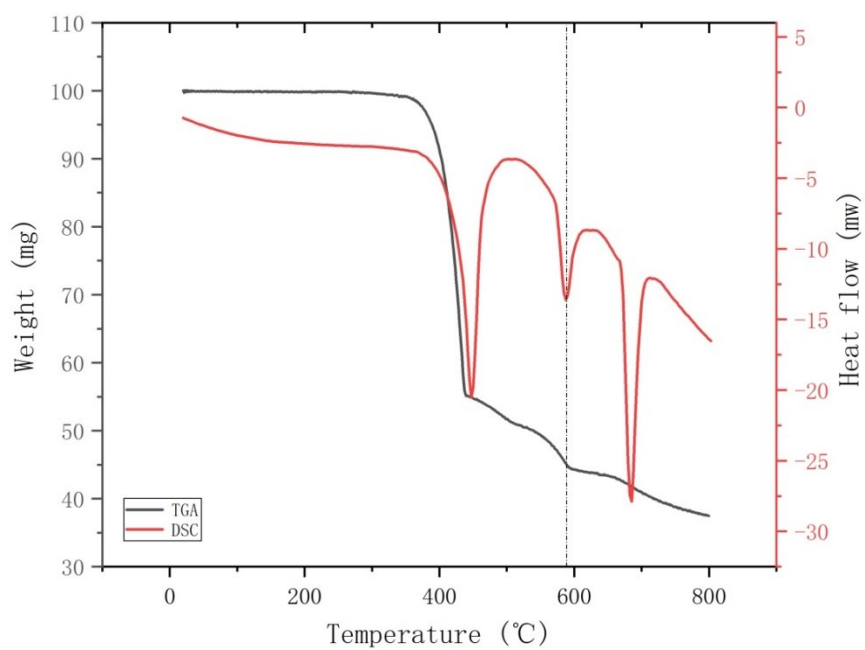


Figure S3. TGA-DSC result of BiSI sample.

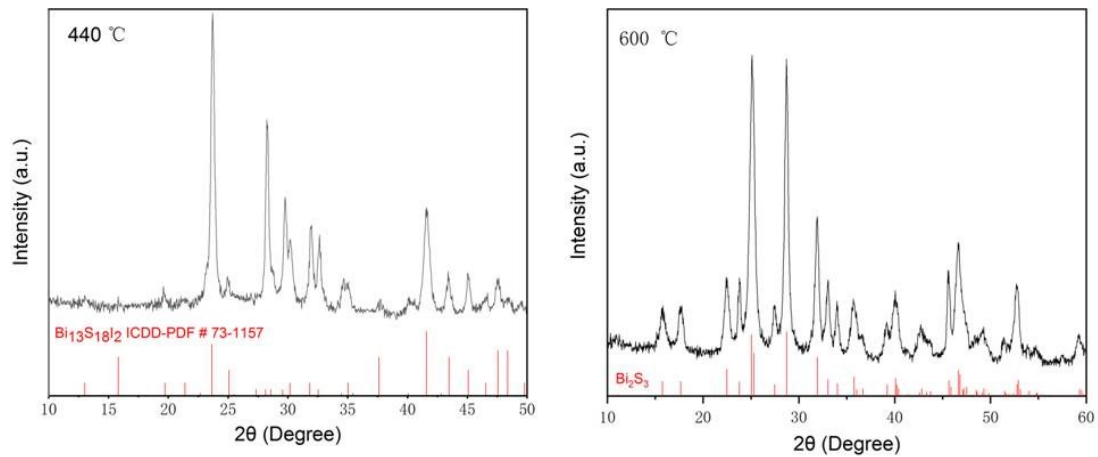


Figure S4. The PXRD pattern of the BiSI sample after heating to 440 °C and 600 °C, compared with Bi_2S_3 (ICDD PDF 75-1306).

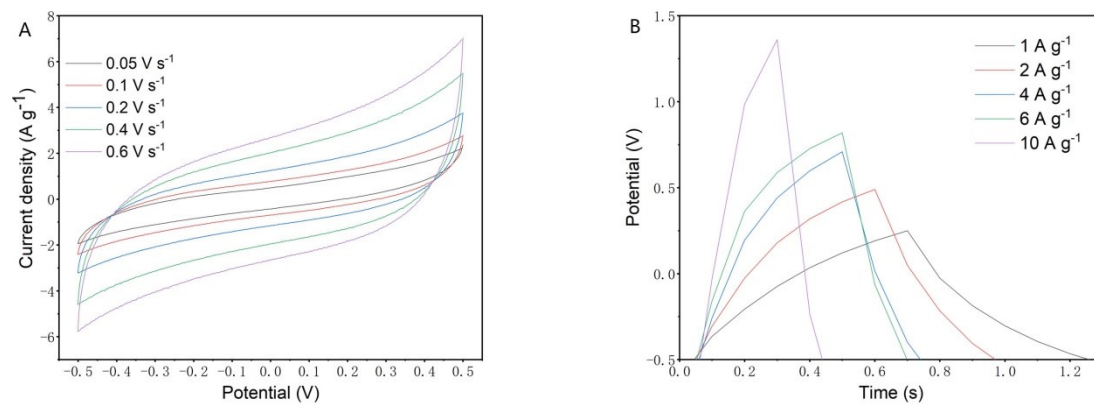


Figure S5. CV and GCD of controlled experiment.

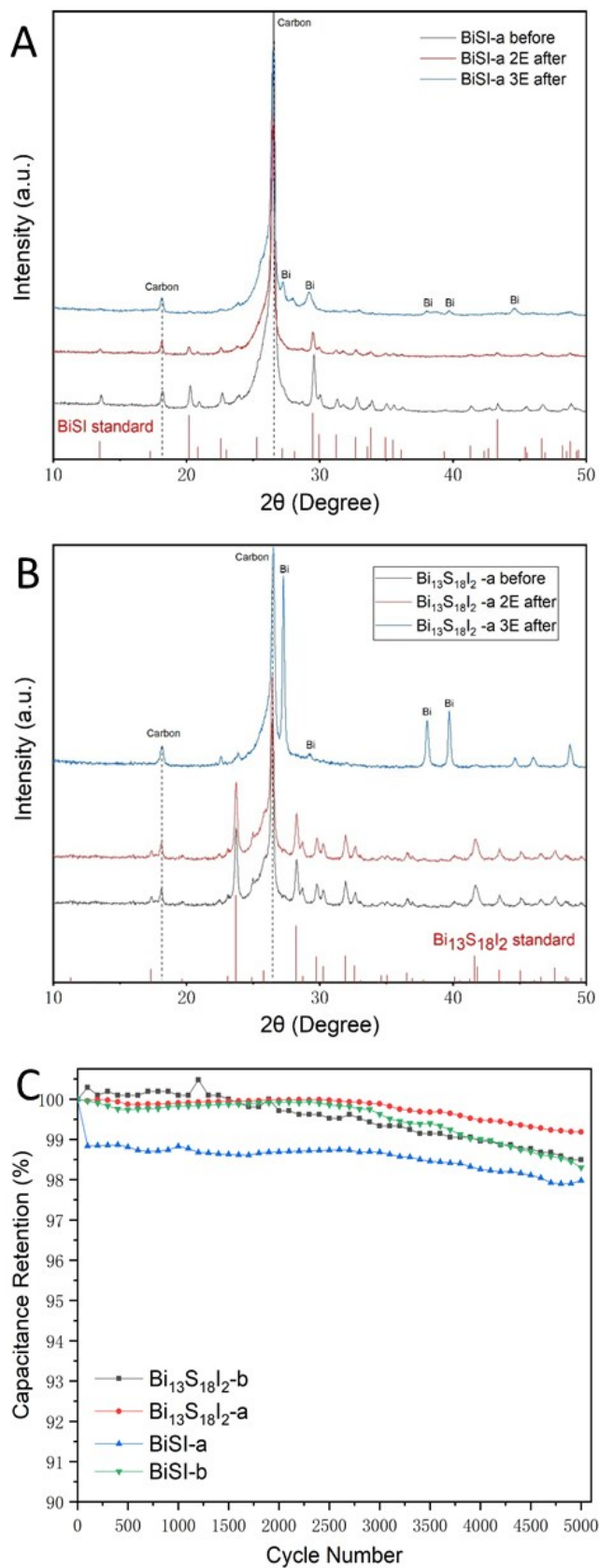


Fig S6. XRD compare of 2E and 3E. (A) BiSI ICDD PDF card No. 43-652, (B) Bi₁₃S₁₈I₂ ICDD PDF card No. 73-1157. (C) The stability comparison of four electrodes during 5000 cycles in EDLC system.

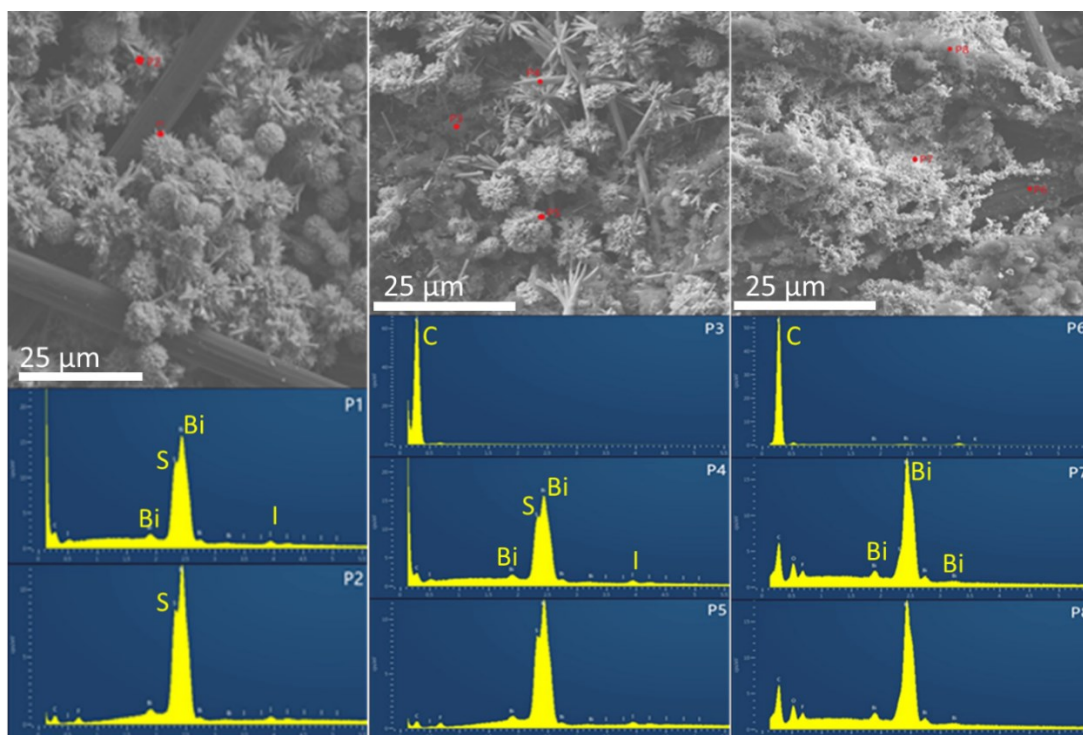


Figure S7a. EDS result of $\text{Bi}_{13}\text{S}_{18}\text{I}_2$ -a electrode before cycle, after 2000 cycles in three electrodes system and after 5000 cycles in two electrodes system (from left to right).

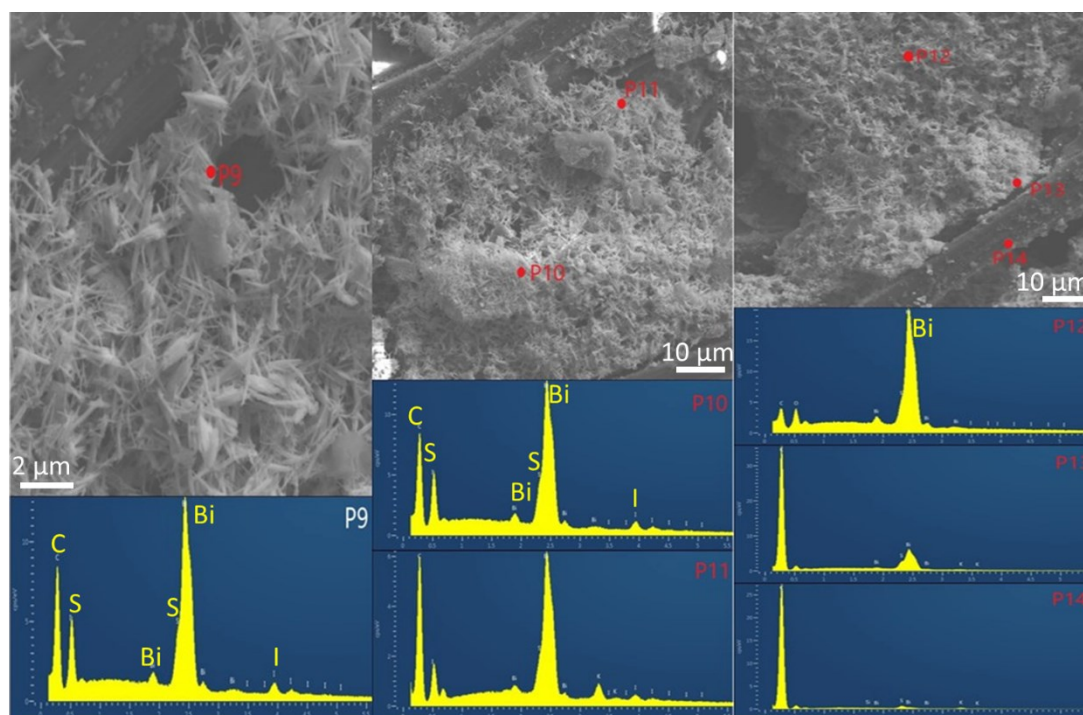


Figure S7b. EDS result of BiSI -b electrode before cycle, after 2000 cycles in three electrodes system and after 5000 cycles in two electrodes system (from left to right).

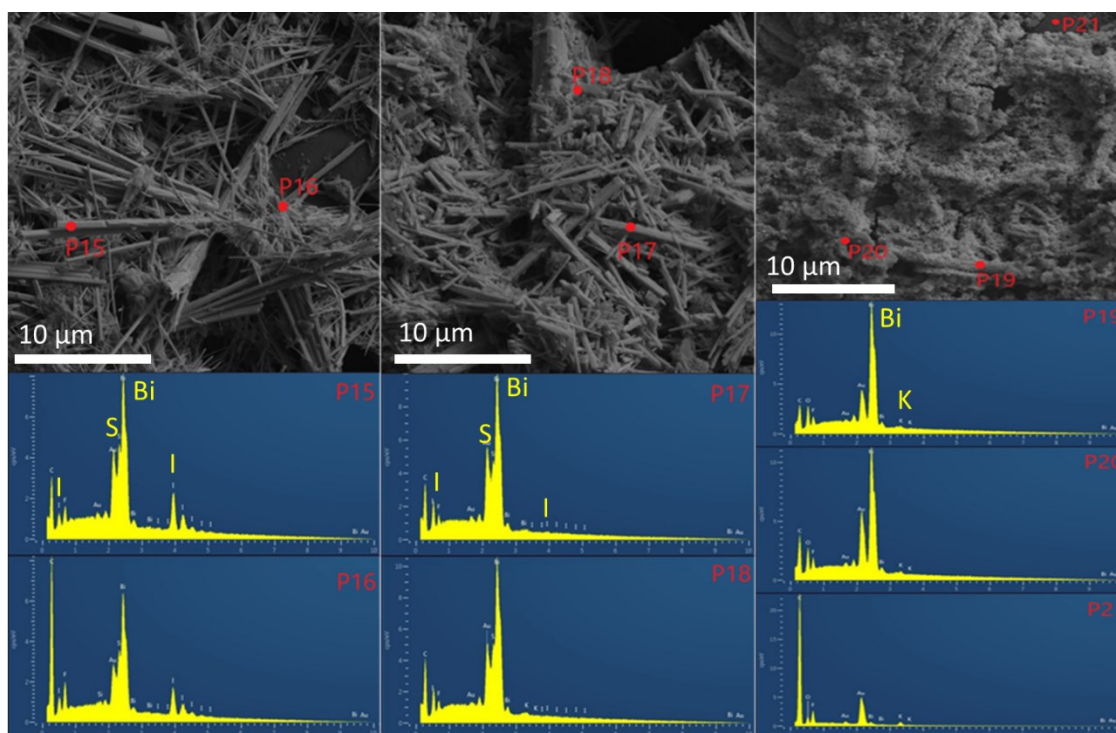


Figure S7c. EDS result of BiSI-a electrode before cycle, after 2000 cycles in three electrodes system and after 5000 cycles in two electrodes system (from left to right).

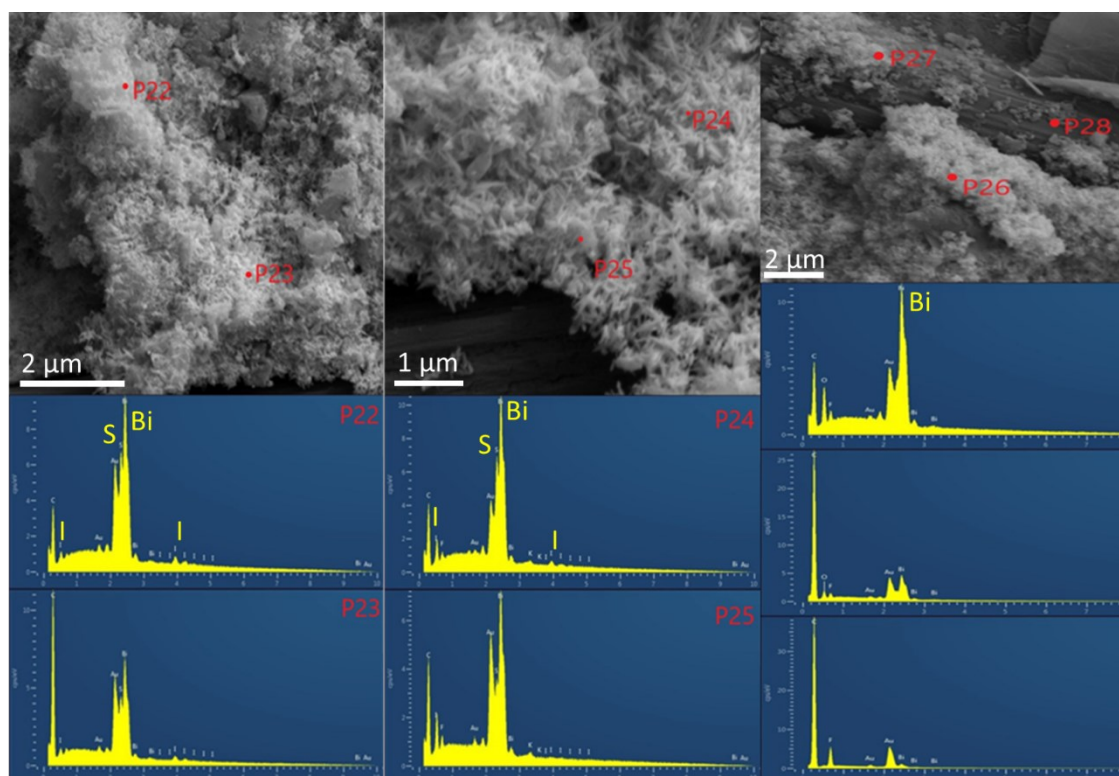


Figure S7d. EDS result of $\text{Bi}_{13}\text{S}_{18}\text{I}_2$ -b electrode before cycle, after 2000 cycles in three electrodes system and after 5000 cycles in two electrodes system (from left to right).