

Solid State Engineering of Bi₂S₃/rGO Nanostrips: An Excellent Electrode Material for Energy Storage Applications

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Optimization of reaction parameters by Response Surface Methodology:

Central Composite design (CCD) of experiments by Design Expert software.

Table S1: Experimental matrix as computed from CCD and responses obtained from XRD phase analyses

Run	Factor 1 A: Temperature dC	Factor 2 B: Time hrs	Factor 3 C:Precursor ratio mole	Response Phase purity
1	153.636	14	4	1
2	120	14	4	0
3	140	16	2	0
4	100	16	6	0
5	120	14	4	0
6	100	12	2	0
7	140	12	2	0
8	120	14	4	0
9	120	17.3636	4	0
10	120	10.6364	4	0
11	120	14	7.36359	1
12	100	12	6	0
13	86.3641	14	4	0
14	120	14	0.636414	0
15	120	14	4	0
16	120	14	4	0
17	120	14	4	0
18	140	16	6	1
19	100	16	2	0
20	140	12	6	1

Analysis

ANOVA for Quadratic model:

$$Y_{response} = \beta_0 + \beta_1A + \beta_2B + \beta_3C + \beta_{12}AB + \beta_{23}BC + \beta_{13}AC + \beta_{11}A^2 + \beta_{22}B^2 + \beta_{33}C^2$$

Response: Phase optimization

Table S2: Estimated values for the optimization of Bi₂S₃ nanorod synthesis using CCD.

Source	Sum of Squares	df	Mean Square	F-value	p-value	
Model	3.15	9	0.3501	71.34	< 0.0001	significant
A-Temperature	0.9926	1	0.9926	202.26	< 0.0001	
B-Time	4.441E-16	1	4.441E-16	9.049E-14	1.0000	
C-Precursor ratio	0.9926	1	0.9926	202.26	< 0.0001	
AB	4.441E-16	1	4.441E-16	9.049E-14	1.0000	
AC	0.5000	1	0.5000	101.88	< 0.0001	
BC	0.0000	1	0.0000	0.0000	1.0000	
A²	0.3459	1	0.3459	70.48	< 0.0001	
B²	0.0069	1	0.0069	1.40	0.2637	
C²	0.3459	1	0.3459	70.48	< 0.0001	
Residual	0.0491	10	0.0049			
Lack of Fit	0.0491	5	0.0098			
Pure Error	0.0000	5	0.0000			
Cor Total	3.20	19				

Factor coding is **Coded**.

Sum of squares is **Type III - Partial**

The **Model F-value** of 71.34 implies the model is significant. There is only a 0.01% chance that an F-value this large could occur due to noise. **P-values** less than 0.0500 indicate model terms are significant. In this case A, C, AC, A², C² are significant model terms. Values greater than 0.1000 indicate the model terms are not significant. If there are many insignificant model terms (not counting those required to support hierarchy), model reduction may improve your model.

Fit Statistics

Table S3: Statistical values obtained from the ANOVA test.

Std. Dev.	0.0701
Mean	0.2000
C.V. %	35.03
R²	0.9847
Adjusted R²	0.9709
Predicted R²	0.8840
Adeq Precision	22.9933

The **Predicted R²** of 0.8840 is in reasonable agreement with the **Adjusted R²** of 0.9709; i.e., the difference is less than 0.2. **Adeq Precision** measures the signal to noise ratio. A ratio greater than 4 is desirable. Your ratio of 22.993 indicates an adequate signal. This model can be used to navigate the design space.

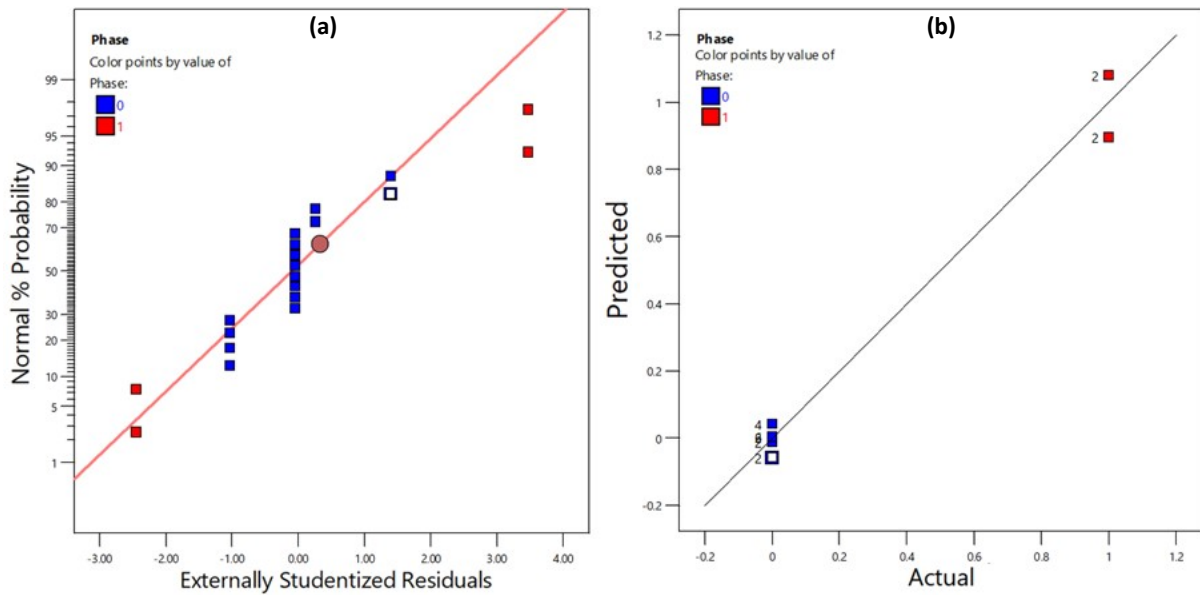


Figure S1: The normal probability plot and the predicted vs actual plot.

Y

$$\begin{aligned}
 &= 0.00334361 + 0.269593 * A + 1.13197 \times 10^{-17} * B + 0.269 \\
 &10^{-18} * AB + 0.25 * AC - 4.20817 \times 10^{-18} * BC + 0.154924 * A \\
 &- 0.021852 * B^2 + 0.154924 * C^2
 \end{aligned}$$

Parameter interaction:

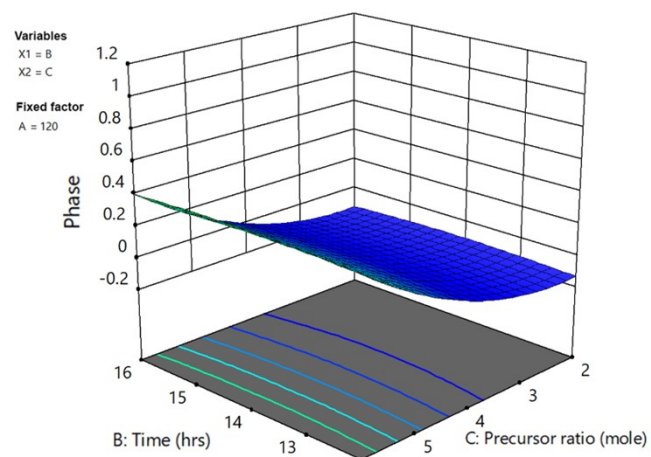
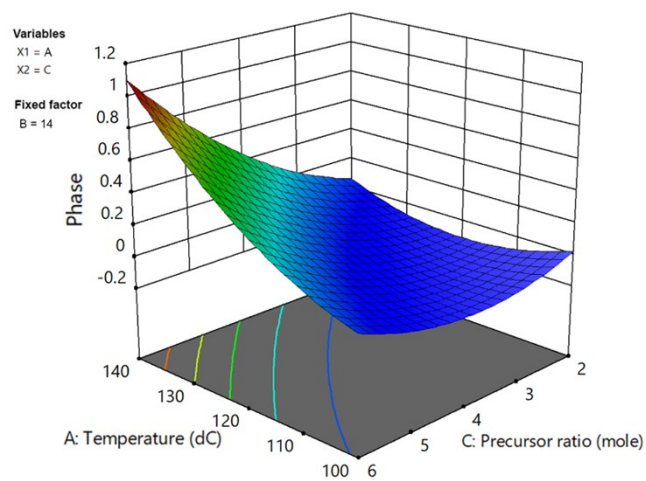
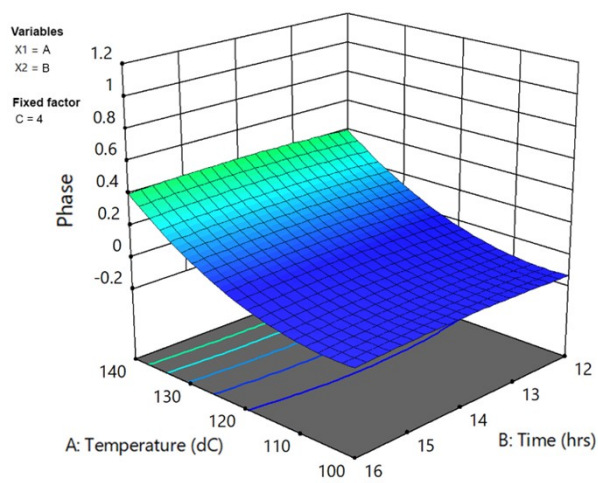


Figure S2: 3D surface plot for two interacting parameters keeping the other constant.

Optimization:

Table S4: List of constrains for the optimization test.

Name	Goal	Lower Limit	Upper Limit	Lower Weight	Upper Weight	Importance
A:Temperature	is in range	100	140	1	1	3
B: Time	is in range	12	16	1	1	3
C:Precursor ratio	is in range	2	6	1	1	3
Phase	maximize	0	1	1	1	3

Solutions

100 Solutions found. The best is selected as marked in blue.

Table S5: List of solutions with optimal reaction parameters for desired result.

Number	Temperature	Time	Precursor ratio	Phase	Desirability	
1	139.061	12.776	5.957	1.038	1.000	Selected
2	139.187	15.927	5.900	1.008	1.000	
3	138.167	14.524	5.965	1.012	1.000	
4	139.187	12.073	5.900	1.008	1.000	
5	140.000	12.000	6.000	1.081	1.000	
6	138.996	15.927	5.919	1.008	1.000	
7	140.000	16.000	6.000	1.081	1.000	
8	138.996	12.073	5.919	1.008	1.000	
9	139.062	15.673	5.912	1.013	1.000	
10	139.663	12.275	5.963	1.057	1.000	
11	138.899	12.689	5.903	1.009	1.000	
12	139.508	15.313	5.950	1.052	1.000	
13	139.025	13.558	5.974	1.051	1.000	
14	139.508	14.423	5.804	1.002	1.000	
15	139.637	12.990	5.811	1.005	1.000	
16	139.561	13.161	5.868	1.027	1.000	
17	139.144	12.246	5.974	1.040	1.000	
18	139.556	13.552	5.810	1.006	1.000	
19	139.825	13.279	5.935	1.066	1.000	
20	139.774	13.243	5.819	1.016	1.000	
21	139.334	15.678	5.947	1.038	1.000	
22	138.894	14.697	5.882	1.007	1.000	
23	138.526	15.687	5.946	1.005	1.000	
24	139.673	12.894	5.960	1.066	1.000	
25	139.898	12.504	5.866	1.031	1.000	
26	139.712	13.589	5.930	1.061	1.000	
27	139.143	12.968	5.991	1.058	1.000	
28	139.433	13.424	5.841	1.013	1.000	
29	139.101	14.907	5.870	1.008	1.000	
30	139.454	15.616	5.874	1.014	1.000	

31	139.050	15.232	5.895	1.012	1.000
32	139.668	13.058	5.867	1.030	1.000
33	139.052	13.816	5.981	1.056	1.000
34	138.792	13.178	5.980	1.041	1.000
35	139.774	15.267	5.832	1.016	1.000
36	139.270	13.444	5.894	1.028	1.000
37	139.091	15.637	5.907	1.013	1.000
38	138.880	14.679	5.935	1.028	1.000
39	139.264	12.273	5.936	1.030	1.000
40	138.881	12.357	5.914	1.007	1.000
41	138.554	13.619	5.990	1.038	1.000
42	138.143	13.185	5.954	1.004	1.000
43	138.979	12.637	5.883	1.003	1.000
44	139.479	15.522	5.978	1.059	1.000
45	139.517	15.198	5.990	1.070	1.000
46	139.076	12.949	5.955	1.040	1.000
47	138.133	13.292	5.965	1.009	1.000
48	139.775	14.498	5.808	1.014	1.000
49	138.393	14.319	5.931	1.009	1.000
50	139.185	15.893	5.925	1.019	1.000
51	139.986	14.132	5.836	1.035	1.000
52	139.948	14.146	5.797	1.017	1.000
53	139.829	14.616	5.989	1.089	1.000
54	139.820	15.842	5.855	1.017	1.000
55	139.494	13.917	5.893	1.038	1.000
56	138.528	15.587	5.978	1.020	1.000
57	139.375	13.038	5.974	1.061	1.000
58	138.468	13.532	5.956	1.021	1.000
59	138.520	13.842	5.924	1.011	1.000
60	139.262	12.466	5.930	1.031	1.000
61	138.415	15.734	5.964	1.007	1.000
62	139.843	12.815	5.907	1.050	1.000
63	138.930	12.909	5.934	1.025	1.000
64	139.050	15.262	5.924	1.024	1.000
65	138.358	12.866	5.947	1.007	1.000
66	139.397	12.543	5.980	1.058	1.000
67	139.449	15.624	5.940	1.041	1.000
68	139.448	12.489	5.862	1.011	1.000
69	138.968	14.937	5.881	1.007	1.000
70	139.753	13.800	5.966	1.078	1.000
71	139.313	14.488	5.826	1.002	1.000
72	139.823	13.830	5.868	1.041	1.000
73	139.915	13.638	5.863	1.042	1.000
74	139.940	14.659	5.866	1.043	1.000
75	138.240	14.652	5.944	1.006	1.000
76	139.103	15.449	5.874	1.003	1.000
77	139.044	12.046	5.908	1.005	1.000
78	138.945	13.793	5.899	1.018	1.000
79	138.263	13.562	5.954	1.012	1.000
80	139.996	13.869	5.855	1.043	1.000
81	139.996	15.802	5.804	1.005	1.000
82	138.748	13.965	5.908	1.014	1.000

83	139.871	14.565	5.885	1.048	1.000
84	138.559	15.998	5.984	1.015	1.000
85	138.983	13.383	5.879	1.010	1.000
86	139.758	13.254	5.946	1.067	1.000
87	139.390	13.154	5.902	1.033	1.000
88	139.319	12.319	5.888	1.013	1.000
89	138.621	12.790	5.914	1.003	1.000
90	138.333	15.081	5.998	1.027	1.000
91	139.384	15.292	5.891	1.023	1.000
92	138.587	15.968	5.962	1.008	1.000
93	138.896	15.007	5.900	1.011	1.000
94	135.888	16.000	6.000	0.916	0.916
95	135.751	12.000	5.968	0.899	0.899
96	140.000	12.001	5.455	0.866	0.866
97	116.527	16.000	6.000	0.320	0.320
98	100.000	14.001	2.000	0.024	0.024
99	100.000	14.036	2.000	0.024	0.024
100	100.000	14.050	2.000	0.024	0.024

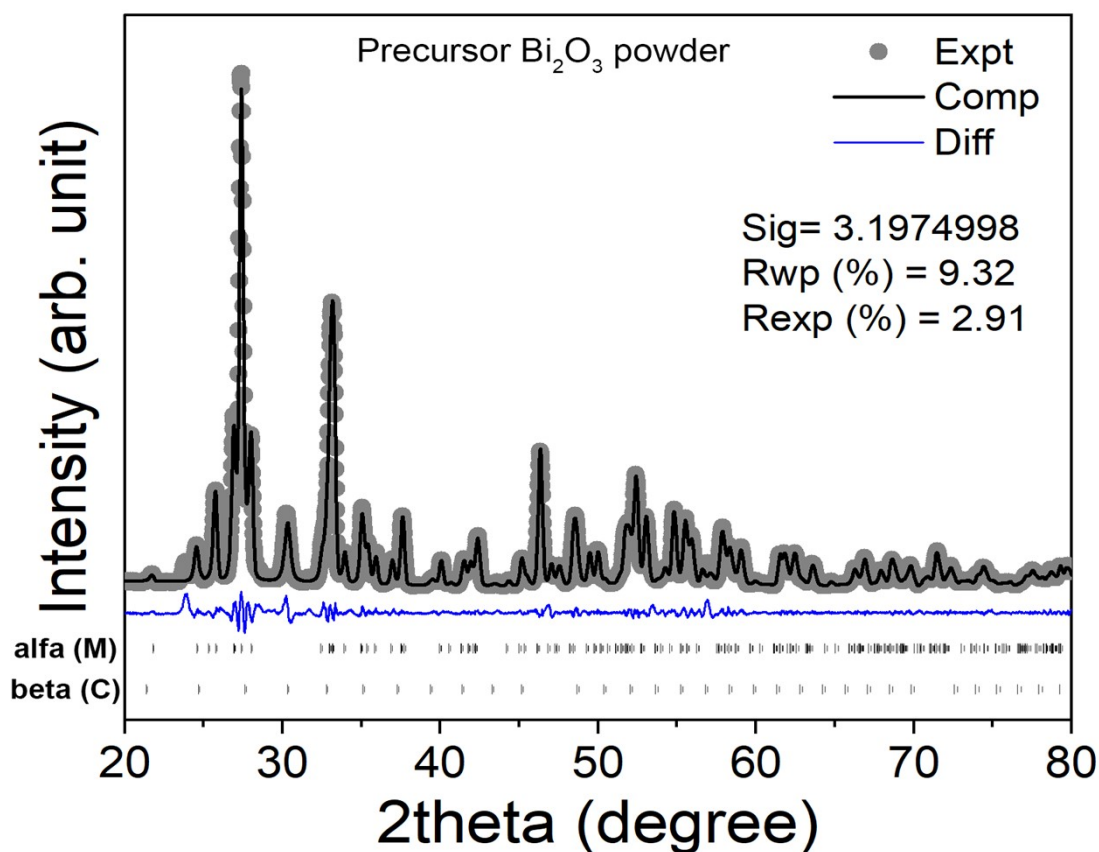


Figure S3: Rietveld refinement of powder X-ray diffraction pattern of precursor Bi_2O_3 powder

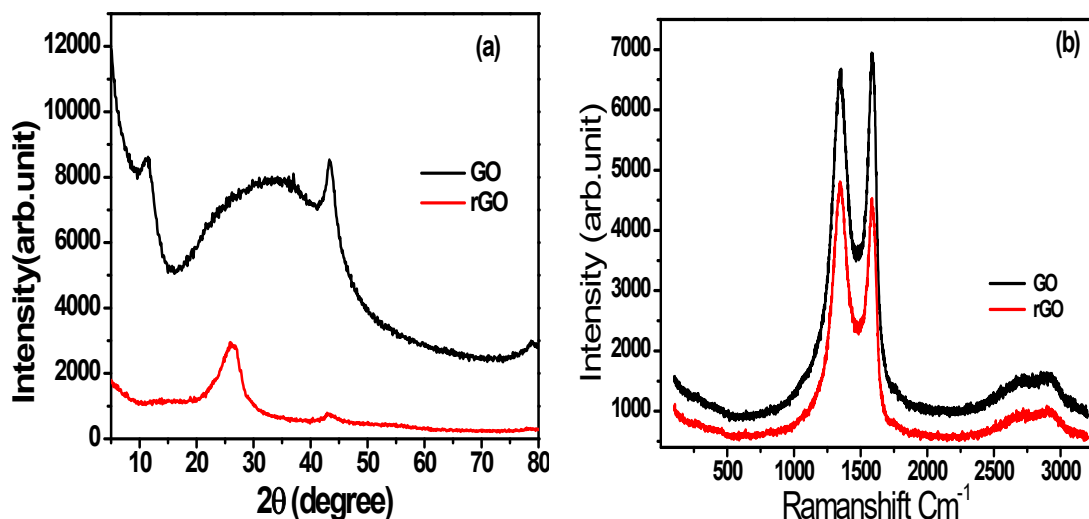


Figure S4: (a) XRD patterns and (b) Raman spectra of GO and rGO samples.

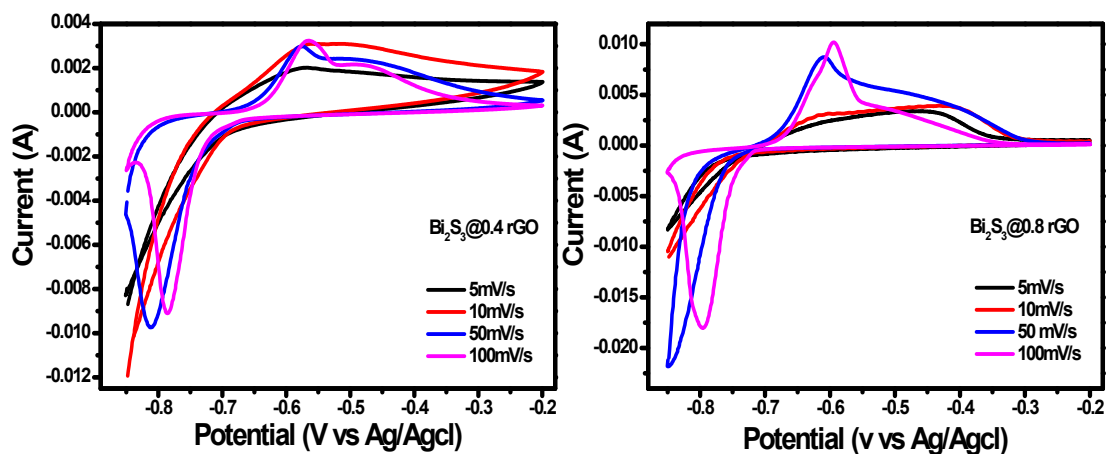


Figure S5: CV measurements of $\text{Bi}_2\text{S}_3@0.4\text{rGO}$ and $\text{Bi}_2\text{S}_3@0.8\text{rGO}$ at different scan rates (5–100 mV/s).

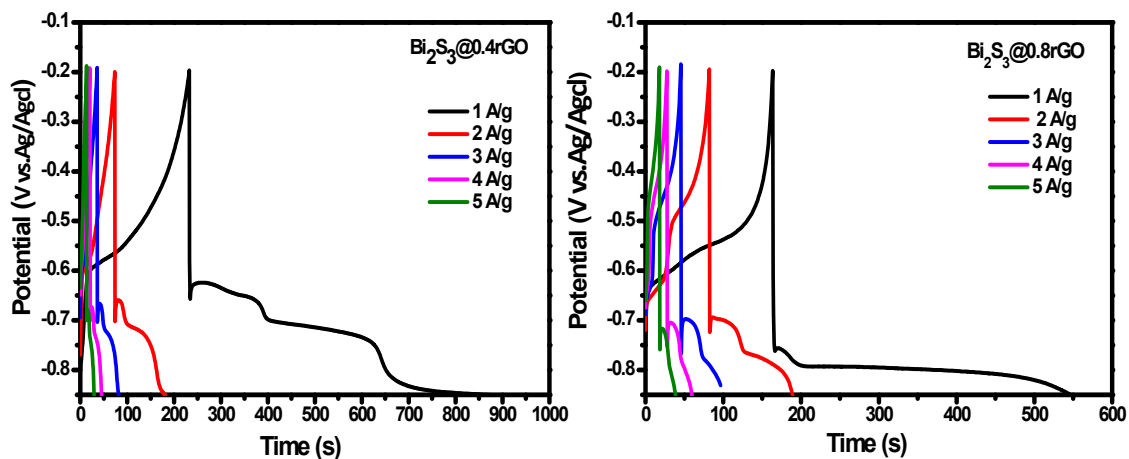


Figure S6: Galvanometric charge-discharge (GCD) of $\text{Bi}_2\text{S}_3@0.4\text{rGO}$ and $\text{Bi}_2\text{S}_3@0.8\text{rGO}$ at different current density 1-5 A/g^{-1} .

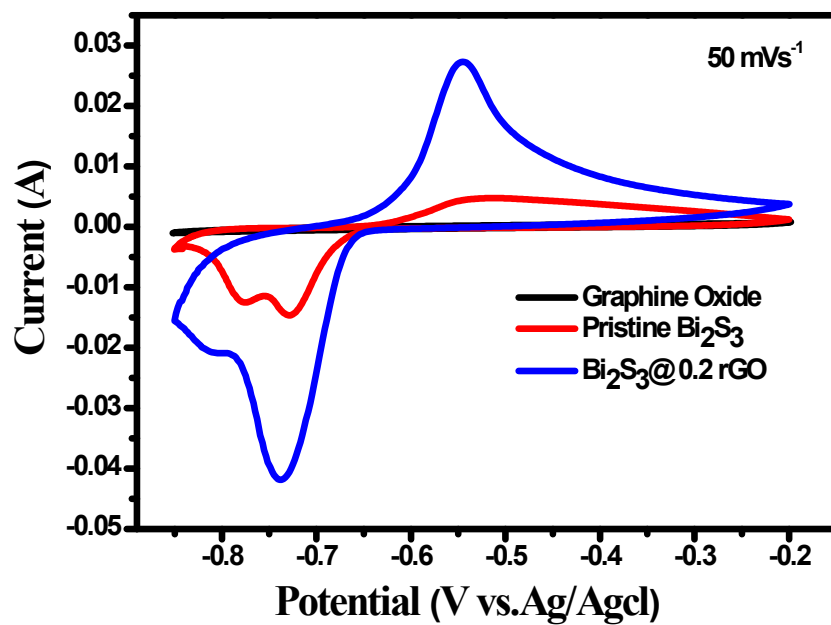


Figure S7: Comparison of CV curves between GO, pristine Bi₂S₃ and Bi₂S₃@0.2rGO nanocomposite.