

*Supplementary Materials*

# Material Design and Optimisation of Electrochemical Li-Ion Storage Properties of Ternary Silicon Oxycarbide/Graphite/Tin Nanocomposites

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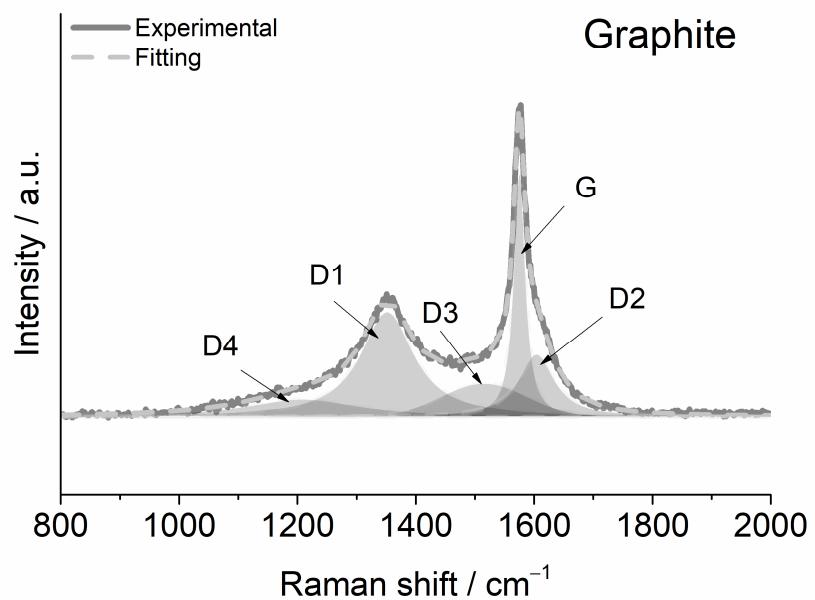
\* Correspondence: monika.wilamowska@pg.edu.pl

**Table S1.** The results of deconvolution of Raman spectra for studied materials.

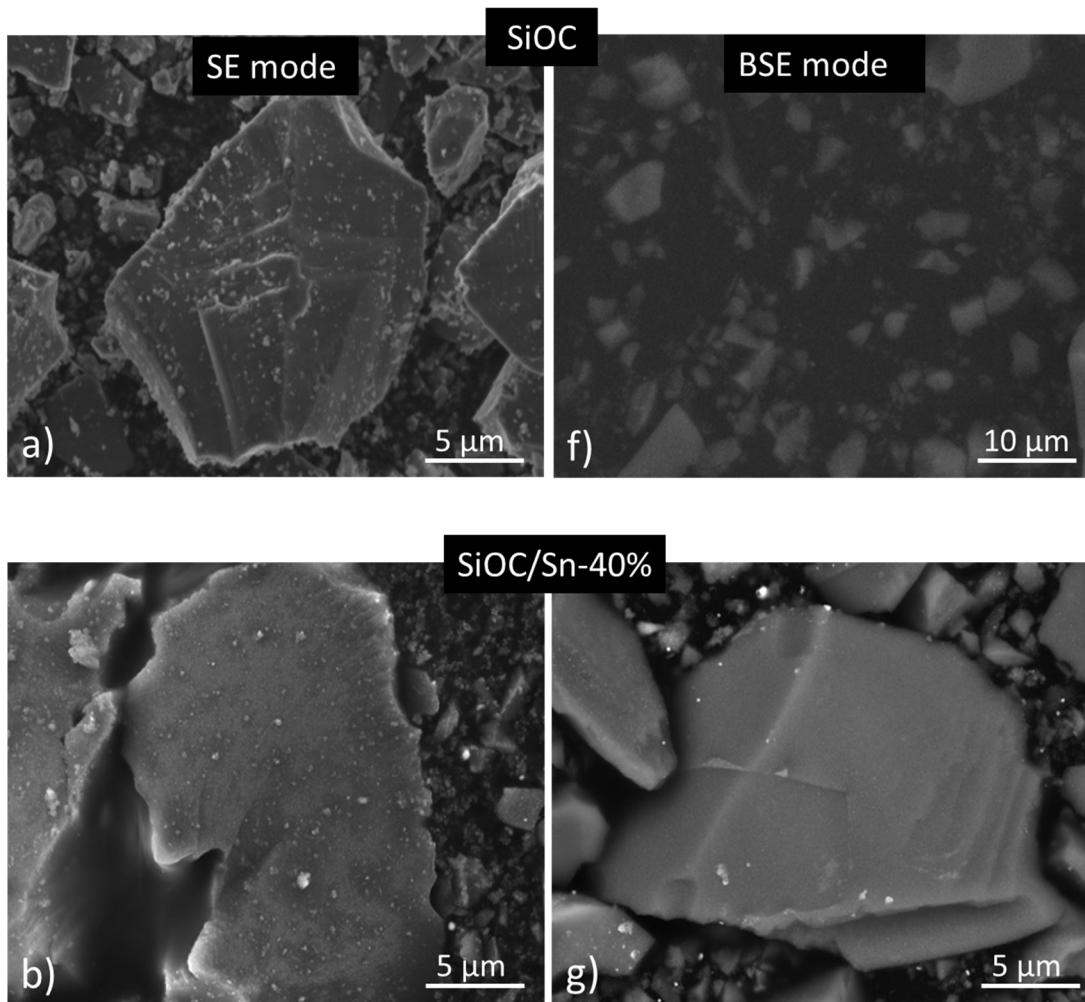
Material	D4		D1		D3		G		D2		$I_{D1}/I_G$	$I_{D2}/I_G$
	cm <sup>-1</sup>	Int.										
<b>Graphite</b>	<b>1209</b>	0.054	1352	0.325	1515	0.103	1575	0.754	1603	0.193	0.431	0.256
SiOC	1210	0.100	1329	0.950	1510	0.223	1572	0.441	1605	0.379	2.154	0.859
SiOC/Sn-40%	1210	0.102	1345	0.881	1520	0.212	1577	0.451	1604	0.347	1.953	0.769
SiOC:C <sub>0.2</sub> /Sn-40%	1260	0.036	1344	0.375	1520	0.112	1576	0.681	1603	0.244	0.551	0.323
SiOC:C <sub>0.2</sub> /Sn-60%	1210	0.064	1342	0.380	1510	0.094	1570	0.790	1603	0.208	0.481	0.263
SiOC:C <sub>0.1</sub> /Sn-60%	1214	0.045	1347	0.493	1519	0.124	1579	0.692	1608	0.351	0.712	0.507

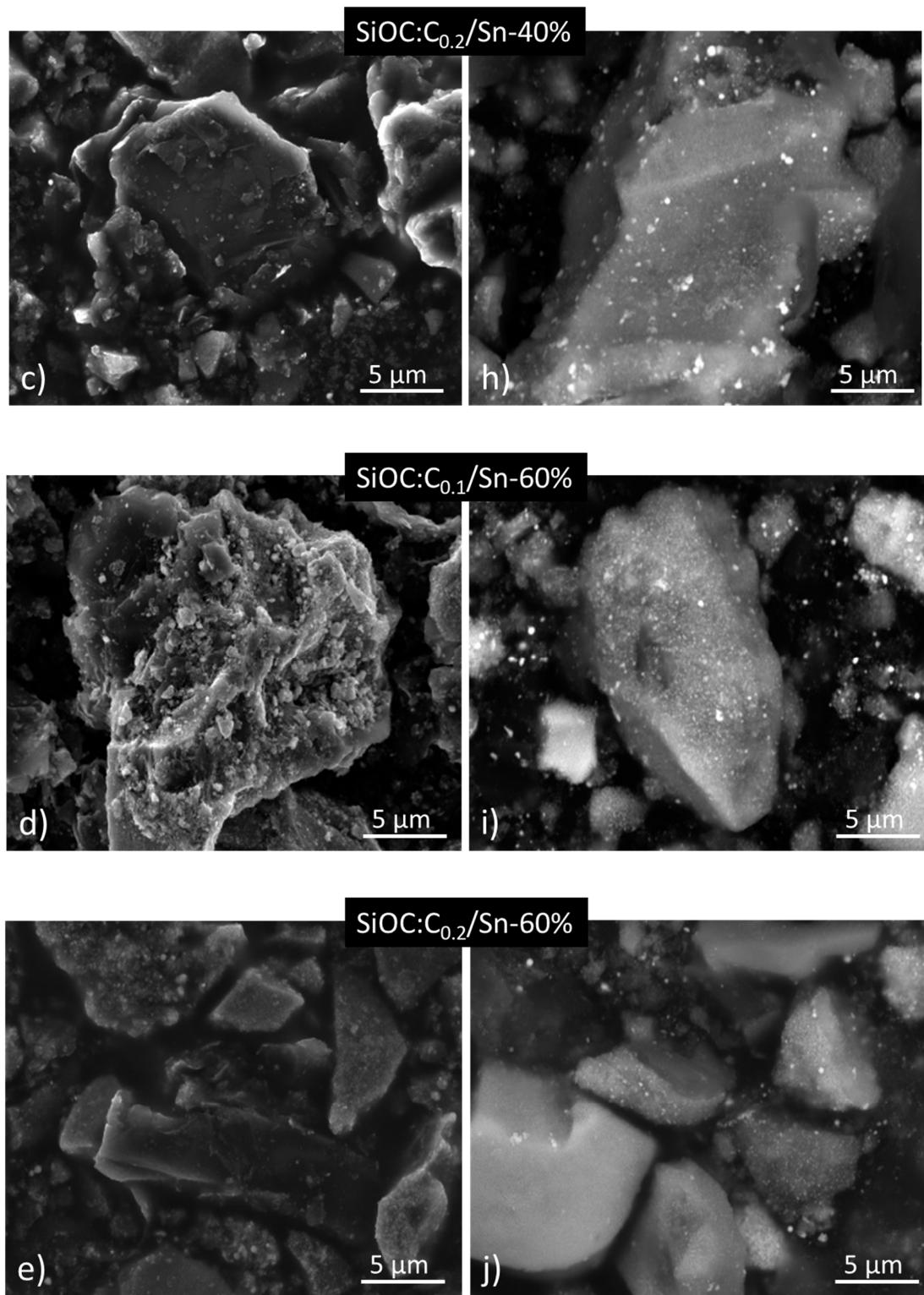
**Table S2.** The results of deconvolution of Raman spectra for studied materials – continuation.

Material	D4		D1		D3		G		D2		
	cm <sup>-1</sup>	Area. %									
Graphite	1209	12.6	1352	38.5	1515	13.8	1575	19.6	1603	15.4	
SiOC	1210	9.3	1329	63.2	1510	8.3	1572	12.5	1605	6.6	
SiOC/Sn-40%	1210	7.8	1345	62.5	1520	8.7	1577	13.2	1604	7.8	
SiOC:C <sub>0.2</sub> /Sn-60%	1210	14.4	1342	41.7	1510	18.9	1570	21.4	1603	10.6	
SiOC:C <sub>0.2</sub> /Sn-40%	1260	3.0	1343	54.1	1520	11.8	1576	14.1	1603	16.9	
SiOC:C <sub>0.1</sub> /Sn -60%	1214	6.1	1347	57.3	1519	8.2	1579	14.1	1608	14.2	

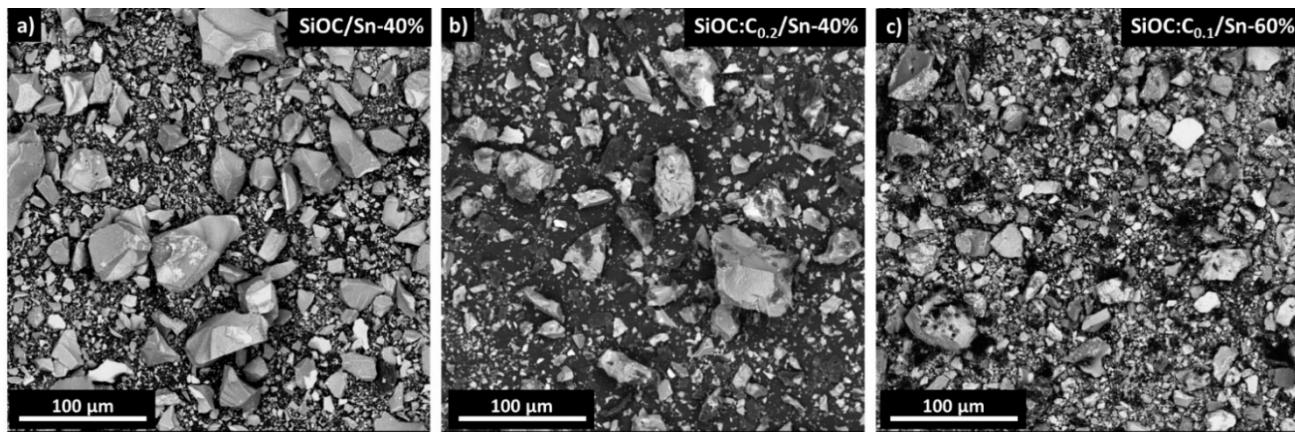


**Figure S1.** Raman fitting results for graphite.

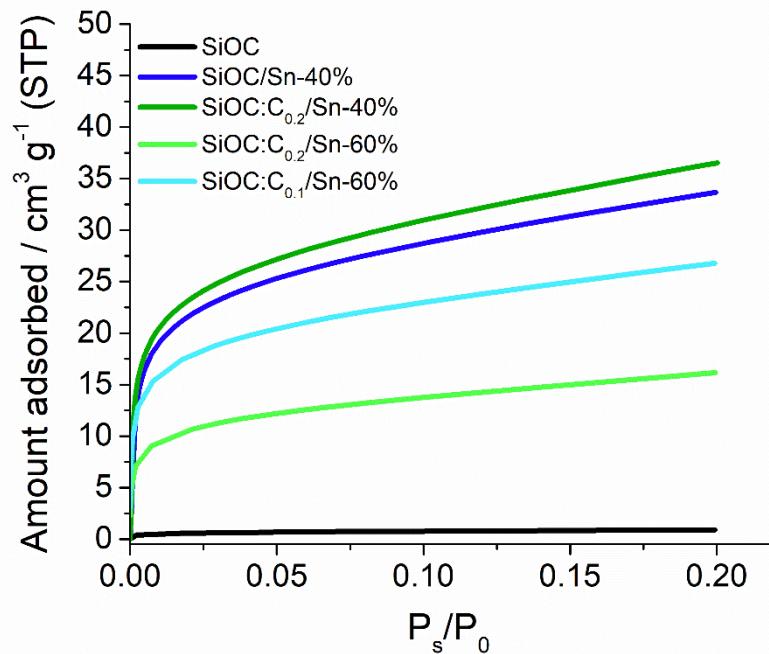




**Figure S2.** SEM images of SiOC, binary SiOC/Sn and ternary SiOC:C/Sn composites, (a–e) secondary electrons mode, (f–j) backscattering mode.



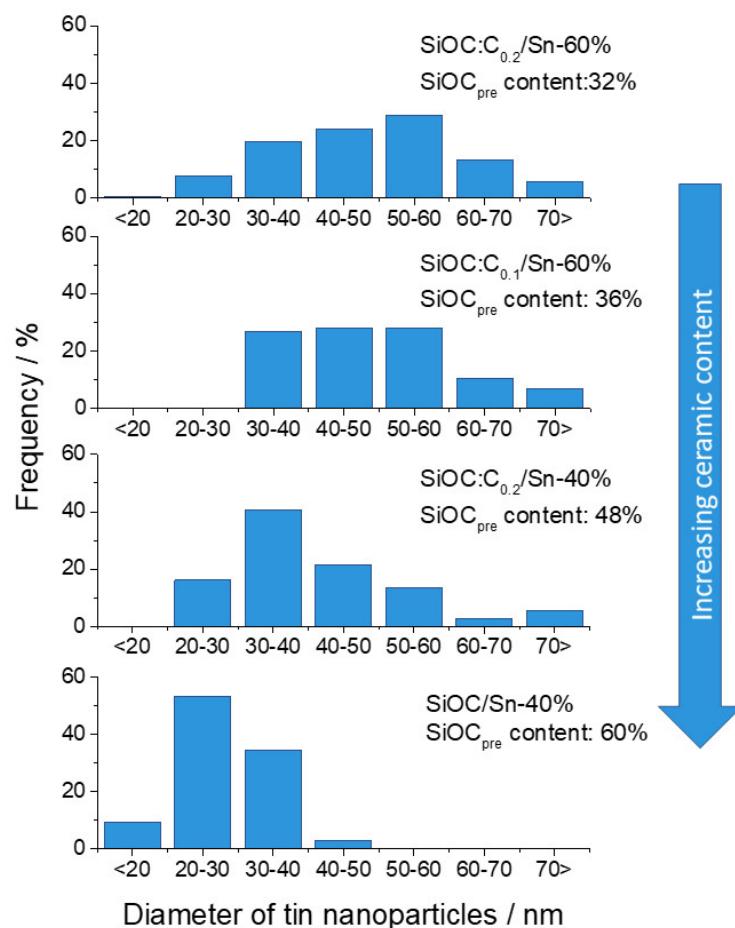
**Figure S3.** SEM images of (a) SiOC/Sn-40%, (b) SiOC:C<sub>0.2</sub>/Sn-40%, and (c) SiOC:C<sub>0.1</sub>/Sn-60% samples.



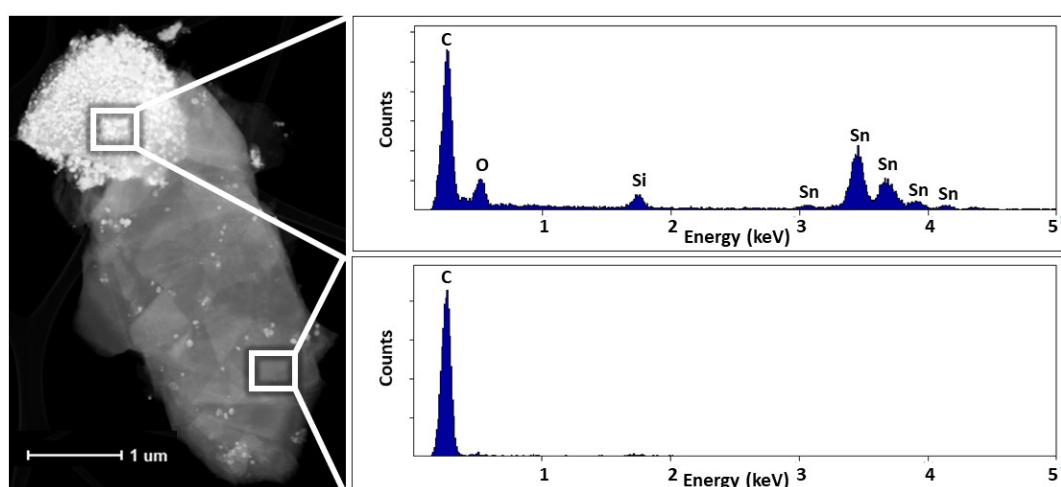
**Figure S4.** The adsorption curves of nitrogen (77 K) for obtained composite materials.

**Table S3.** BET surface area for obtained composite materials.

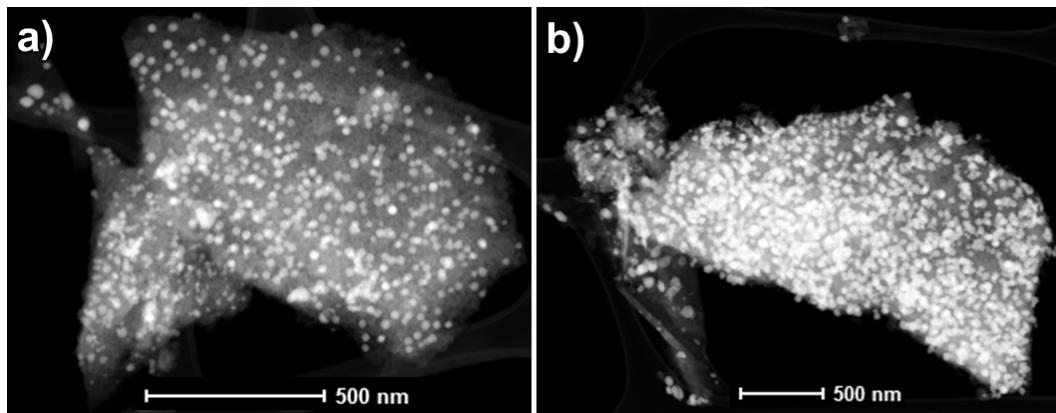
Sample composition	BET surface area [m <sup>3</sup> /g]
SiOC	3.18
SiOC/Sn-40%	118.2
SiOC:C <sub>0.2</sub> /Sn-40%	106.9
SiOC:C <sub>0.2</sub> /Sn-60%	55.1
SiOC:C <sub>0.1</sub> /Sn-60%	94.7



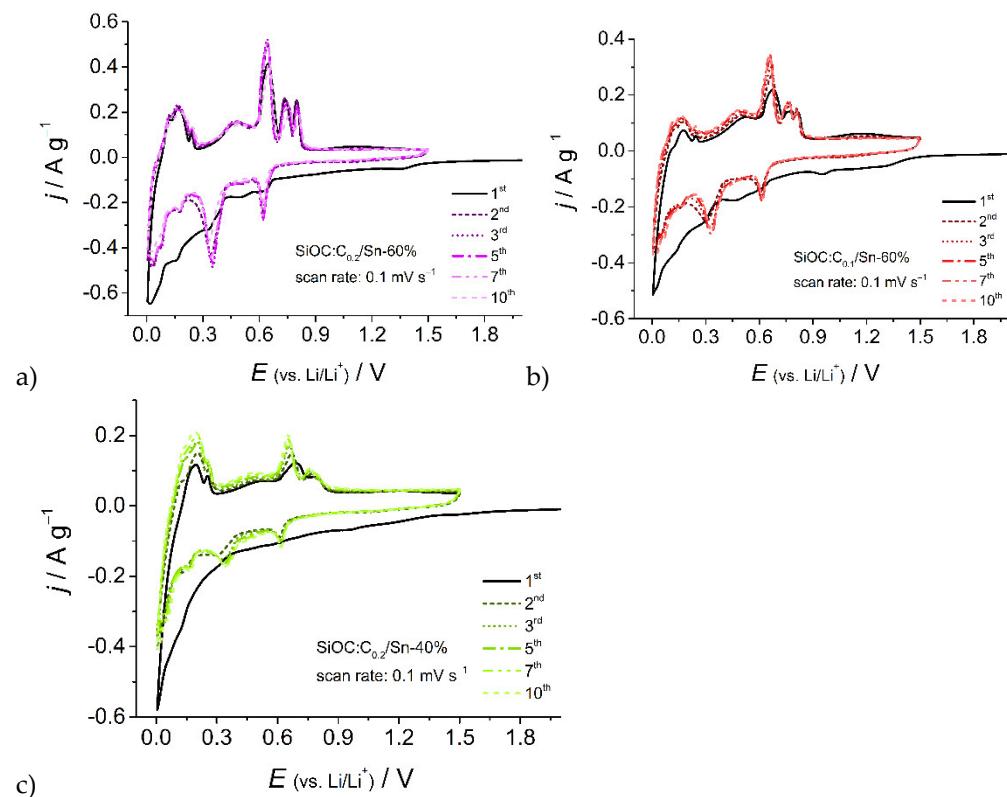
**Figure S5.** The size distribution of the Sn nanoparticles in the SiOC:C/Sn and SiOC/Sn nanocomposites. SiOC<sub>Pre</sub> content corresponds to the weight percentage content of preceramic polymer in preceramic blend.



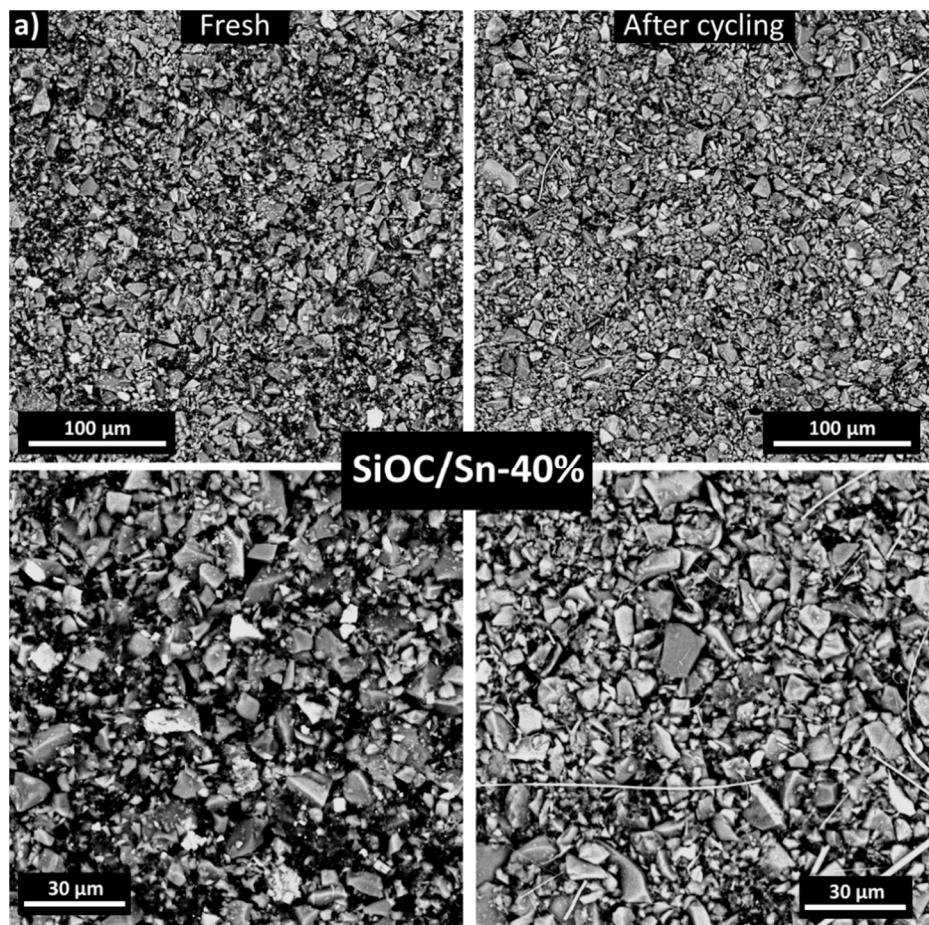
**Figure S6.** EDX elemental composition of tin-rich (SiOC) and tin-poor (graphite) regions of the SiOC:C<sub>0.2</sub>/Sn-60% sample.

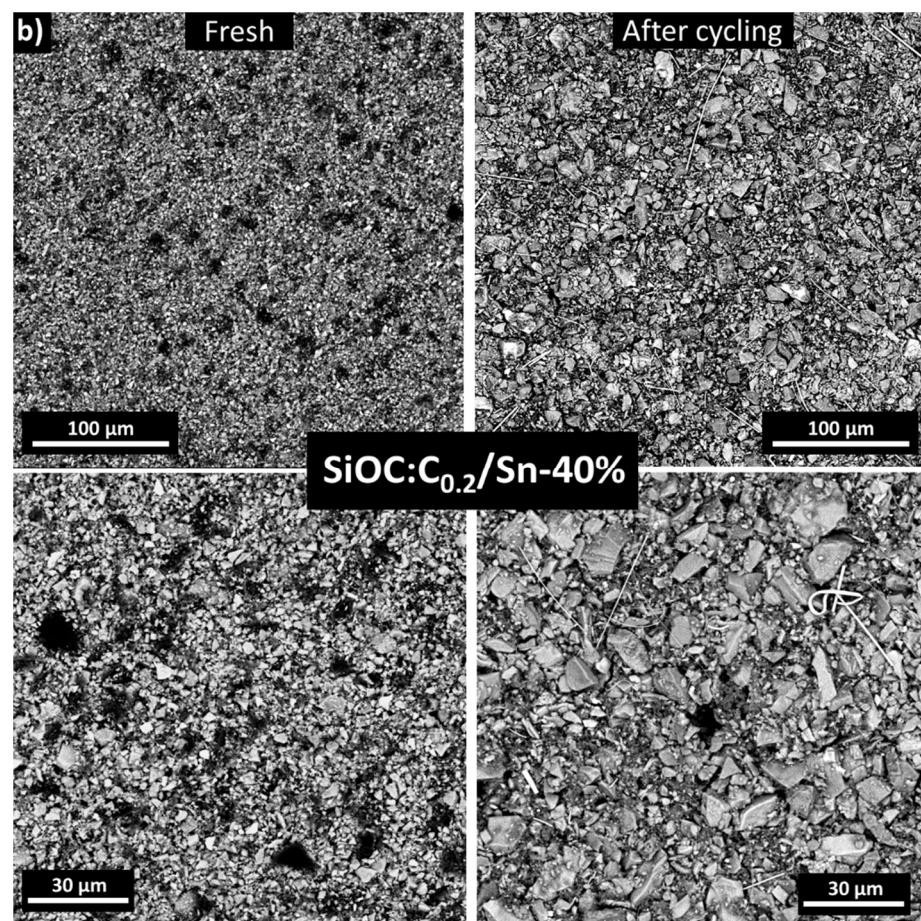


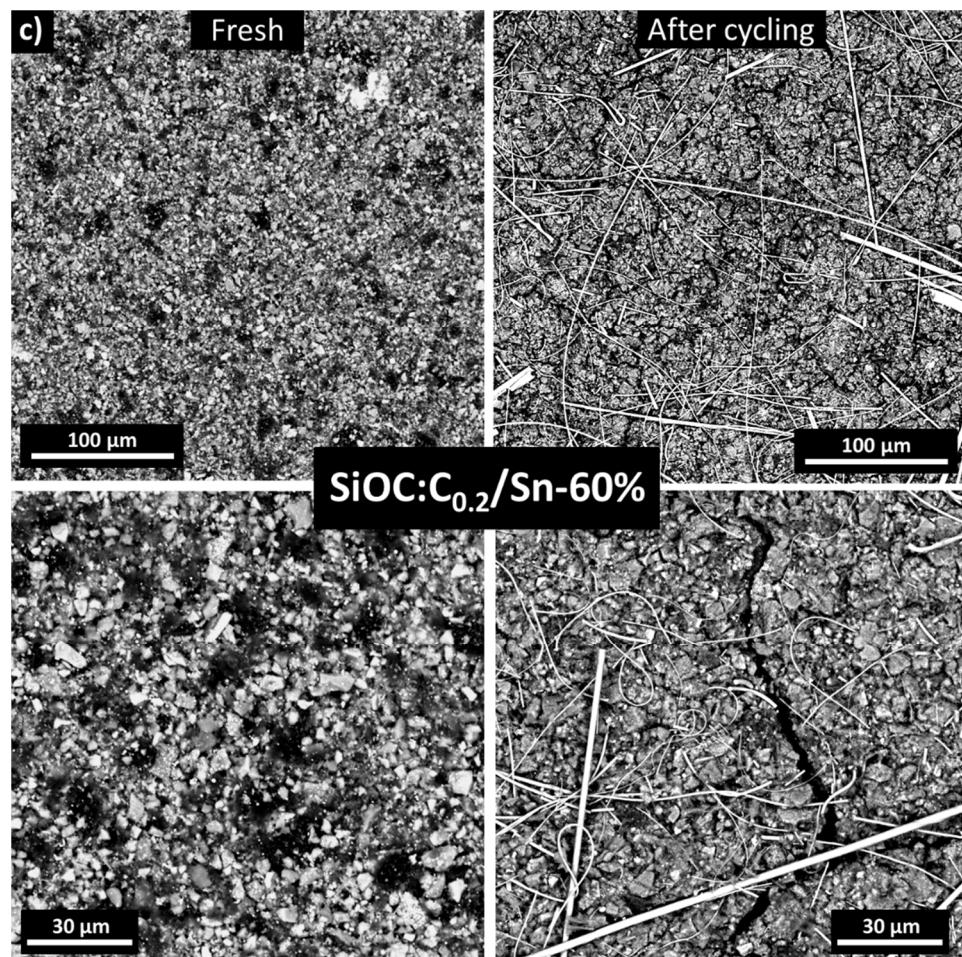
**Figure S7.** SEM images of (a) SiOC:C<sub>0.2</sub>/Sn-40% and (b) SiOC:C<sub>0.1</sub>/Sn-60% composites showing accumulation of tin nanoparticles in the ceramic phase.



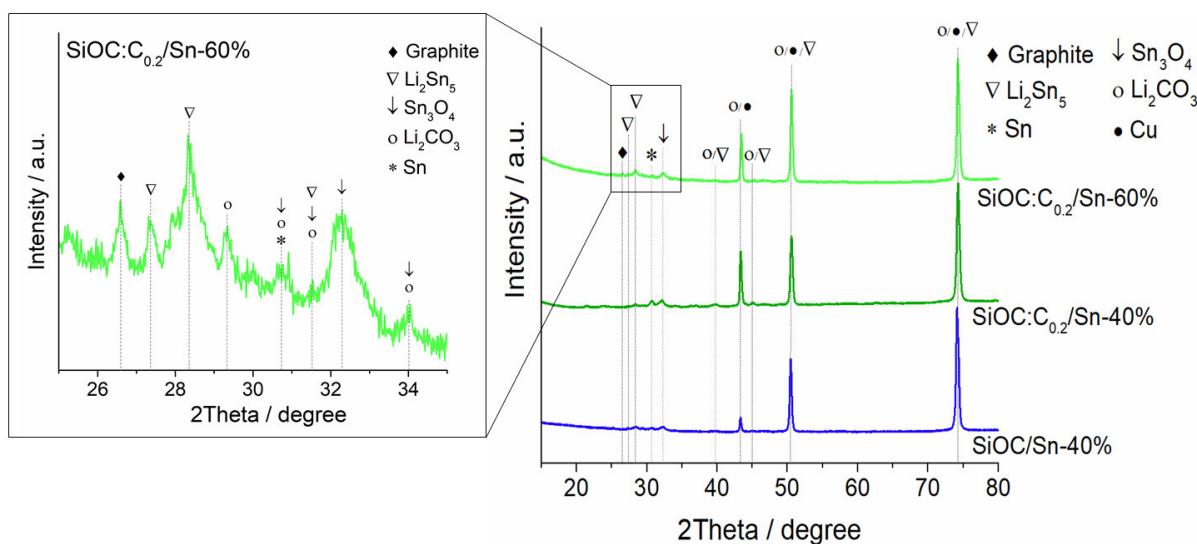
**Figure S8.** Cyclic voltammetry curves of (a) SiOC:C<sub>0.2</sub>/Sn-60%, (b) SiOC:C<sub>0.1</sub>/Sn-60% and (c) SiOC:C<sub>0.2</sub>/Sn-40%.







**Figure S9.** SEM images of electrode layers before ("fresh") and after extended cycling tests (2 cycles at  $18.6 \text{ mA g}^{-1}$  followed by 100 cycles at  $372 \text{ mA g}^{-1}$ ) recorded for (a) SiOC/Sn-40%, (b) SiOC:C<sub>0.2</sub>/Sn-40% and (c) SiOC:C<sub>0.2</sub>/Sn-60%.



**Figure S10.** Diffractograms of the cycled electrodes, Inset: the selected 2Theta range of the diffractogram of SiOC:C<sub>0.2</sub>/Sn-60% composite.

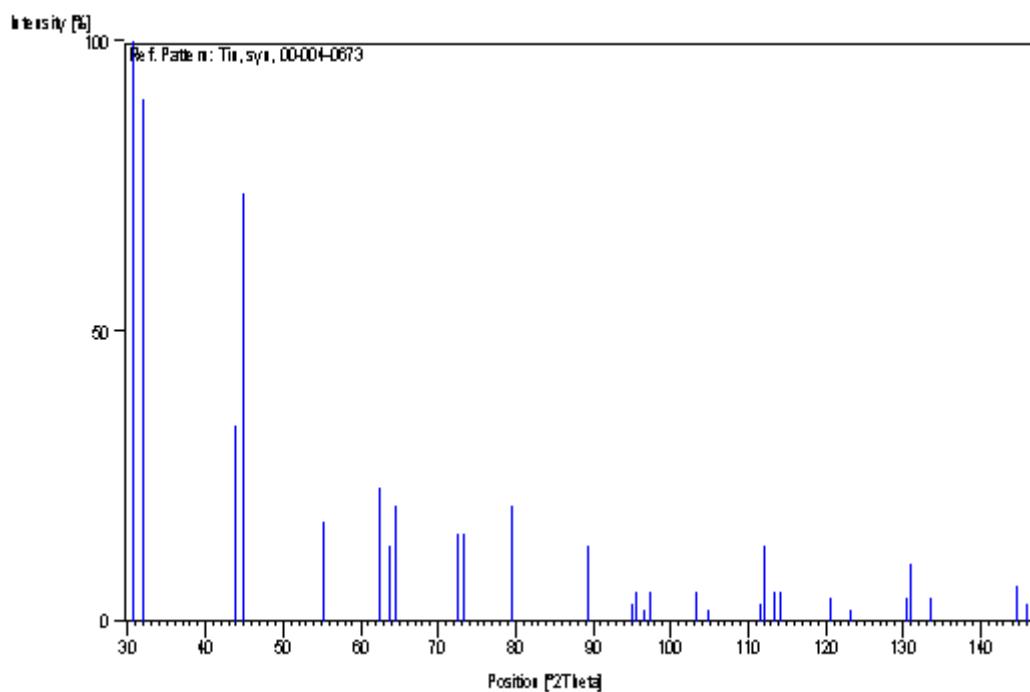
**Table S4.** Data obtained from XRD according to PDF card Sn-ref\_00-004-0673.

<b>Name and formula</b>	
Reference code:	00-004-0673
Mineral name:	Tin, syn
PDF index name:	Tin
Empirical formula:	Sn
Chemical formula:	Sn
<b>Crystallographic parameters</b>	
Crystal system:	Tetragonal
Space group:	I41/amd
Space group number:	141
a (Å):	5.8310
b (Å):	5.8310
c (Å):	3.1820
Alpha (°):	90.0000
Beta (°):	90.0000
Gamma (°):	90.0000
Calculated density (g/cm <sup>3</sup> ):	7.29
Volume of cell (10 <sup>6</sup> pm <sup>3</sup> ):	108.19
Z:	4.00
RIR:	1.97
<b>Subfiles and Quality</b>	
Subfiles:	Inorganic Mineral Alloy, metal or intermetallic Common Phase Educational pattern Forensic NBS pattern
Quality:	Star (S)
<b>Comments</b>	
Color:	Light gray metallic
General comments:	Space group given by Mark, Polanyi, Z. <i>Phys.</i> , <b>18</b> 75-96 (1925). Color from <i>Dana's System of Mineralogy</i> , 7th Ed., 485.
Sample source:	Sample was furnished by Johnson Matthey Company, Ltd. and annealed

	12 hours at 160 C.					
	Analysis (wt.%): Pb 0.0012, Sb 0.001, Fe 0.00027, Cu 0.0002, As 0.0002, Bi 0.00012, S 0.0003, Sn 99.997 (by difference), other form a-Sn (cubic).					
Analysis:						
Additional pattern:	See ICSD 40037 (PDF 86-2264).					
Melting point:	231.8°					
Temperature:	Pattern taken at 26 C					
<b>Peak list</b>						
No	h	k	l	d [Å]	2Theta[deg]	I [%]
1	2	0	0	2.91500	30.645	100.0
2	1	0	1	2.97300	32.019	90.0
3	2	2	0	2.06200	43.872	34.0
4	2	1	1	2.01700	44.903	74.0
5	3	0	1	1.65900	55.332	17.0
6	1	1	2	1.48400	62.540	23.0
7	4	0	0	1.45800	63.785	13.0
8	3	2	1	1.44200	64.578	20.0
9	4	2	0	1.30400	72.416	15.0
10	4	1	1	1.29200	73.198	15.0
11	3	1	2	1.20500	79.472	20.0
12	4	3	1	1.09500	89.412	13.0
13	1	0	3	1.04340	95.167	3.0
14	3	3	2	1.04010	95.565	5.0
15	4	4	0	1.03090	96.699	2.0
16	5	2	1	1.02520	97.418	5.0
17	2	1	3	0.98240	103.275	5.0
18	6	0	0	0.97180	104.868	2.0
19	3	0	3	0.93100	111.663	3.0
20	5	1	2	0.92860	112.101	13.0
21	6	2	0	0.92190	113.348	5.0
22	6	1	1	0.91780	114.130	5.0
23	3	2	3	0.88680	120.599	4.0
24	5	4	1	0.87550	123.246	2.0
25	4	1	3	0.84850	130.416	4.0
26	5	3	2	0.84660	130.976	10.0
27	6	3	1	0.83860	133.431	4.0
28	6	4	0	0.80860	144.590	6.0

29	7	0	1	0.80580	145.859	3.0
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### Stick Pattern



### References

1. Swanson, T. *Natl. Bur. Stand. (U.S.), Circ.* **1953**, 539 I, 24.