

Supplementary Information

Sn-based alloys synthesized in room temperature ionic liquid: Cu_6Sn_5 as a case study

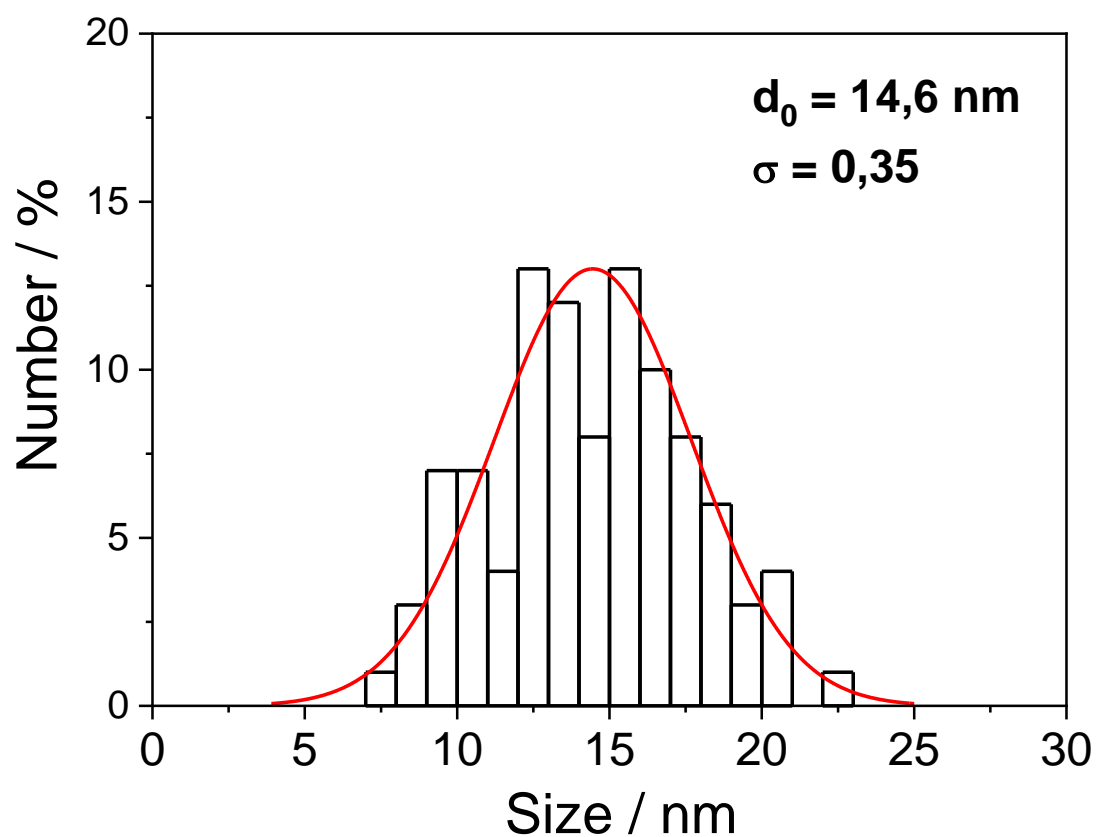


Figure S1. Particle size distribution of β -Sn synthesized using $\text{Sn}(\text{TFSI})_2$ as precursor.

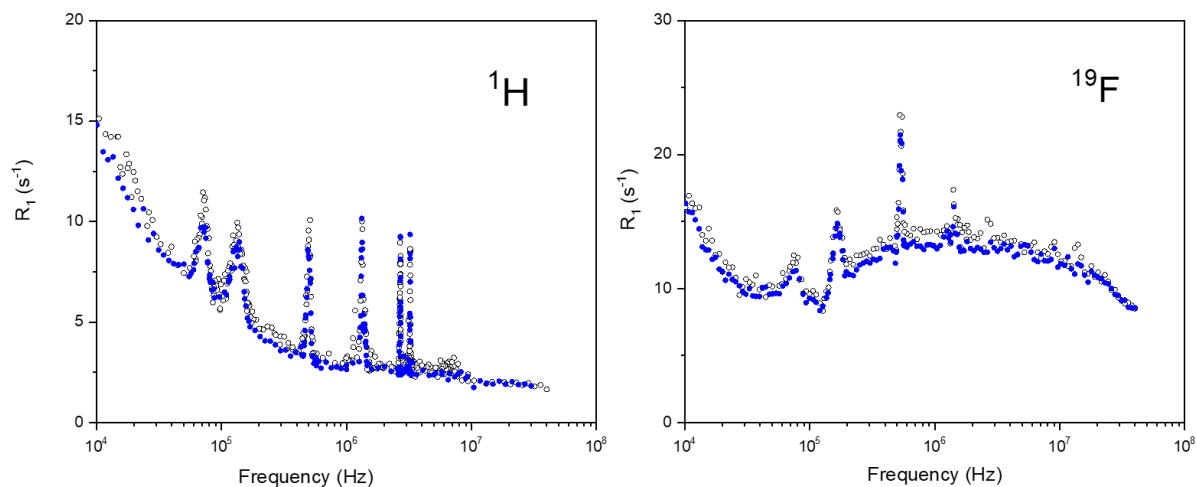


Figure S2. ^1H and ^{19}F spin lattice relaxation rates, R_1 , as a function of the frequency for frozen $[\text{EMIm}^+][\text{TFSI}^-]$ (open symbol) and oxidized Sn nanoparticles in $[\text{EMIm}^+][\text{TFSI}^-]$ (blue symbol).

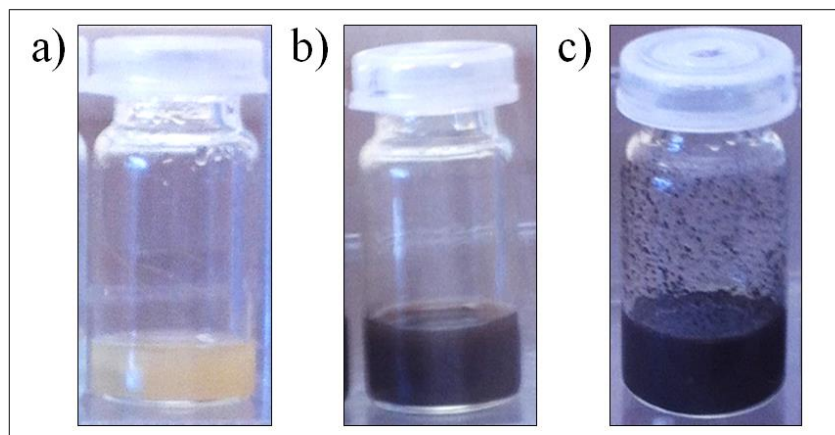


Figure S3. Photographs of $[\text{EMIm}^+][\text{TFSI}^-]$ solutions containing Sn-Cu chlorides (a) and (b), and Sn-Cu TFSI-precursors (c).

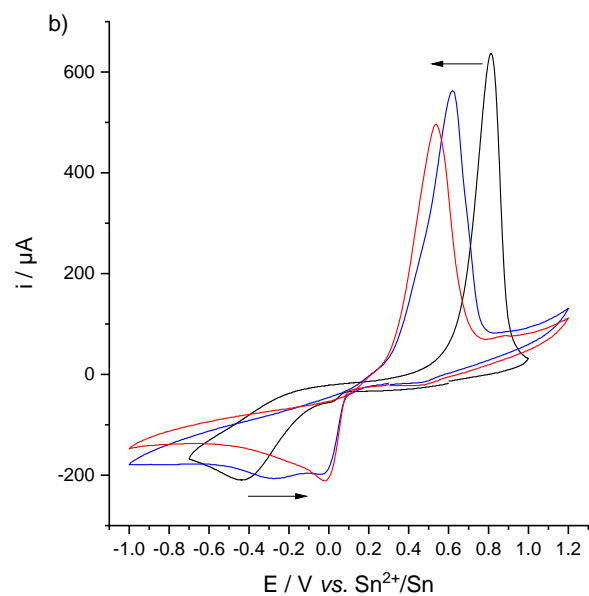


Figure S4. Cyclic voltammograms of a 25 mM of $\text{Cu}(\text{TFSI})_2$ in $[\text{EMIm}^+][\text{TFSI}^-]$. The arrow indicates increasing cycle number.

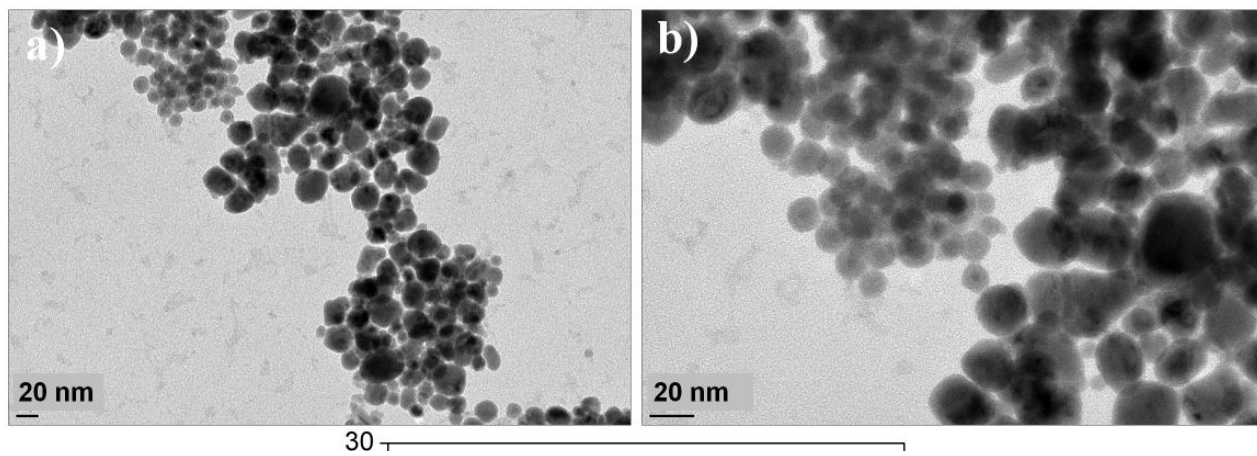


Figure S5. Transmission electron micrographs of Cu-Sn nanoparticles.

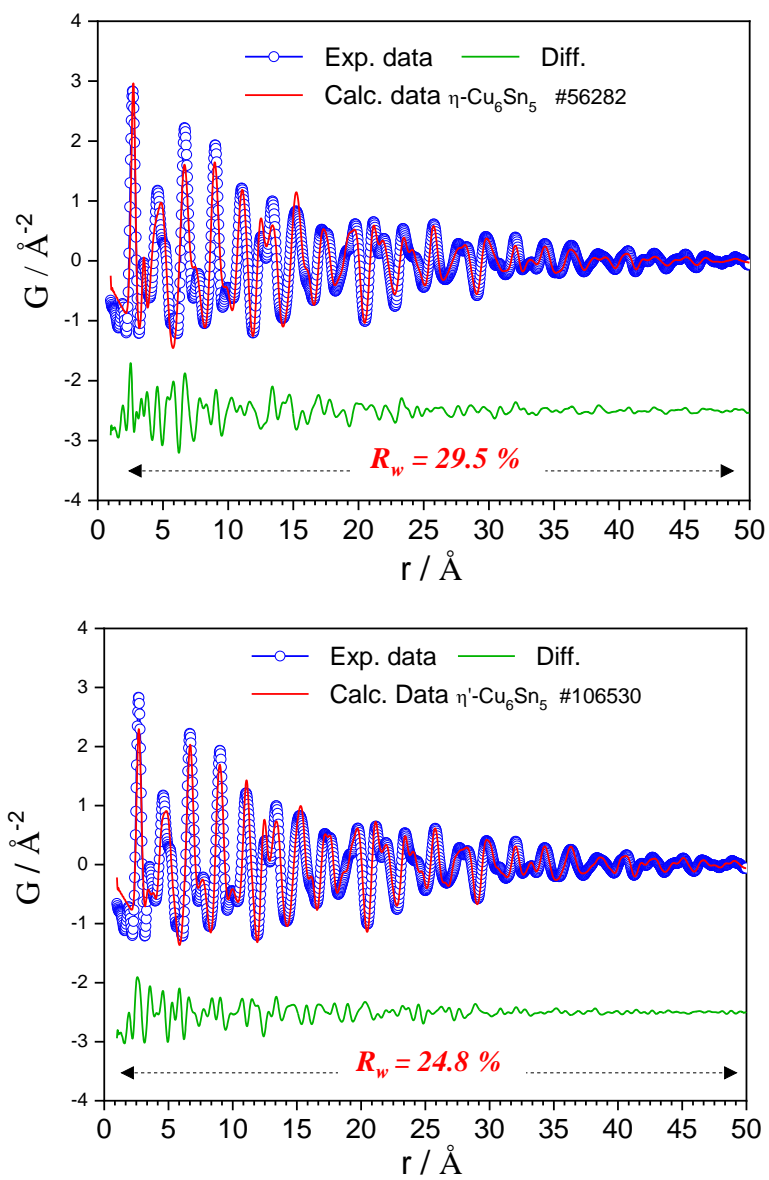


Figure S6. PDF refinements of the as prepared Sn-Cu compound using η and η' - Cu_6Sn_5 as structural models.

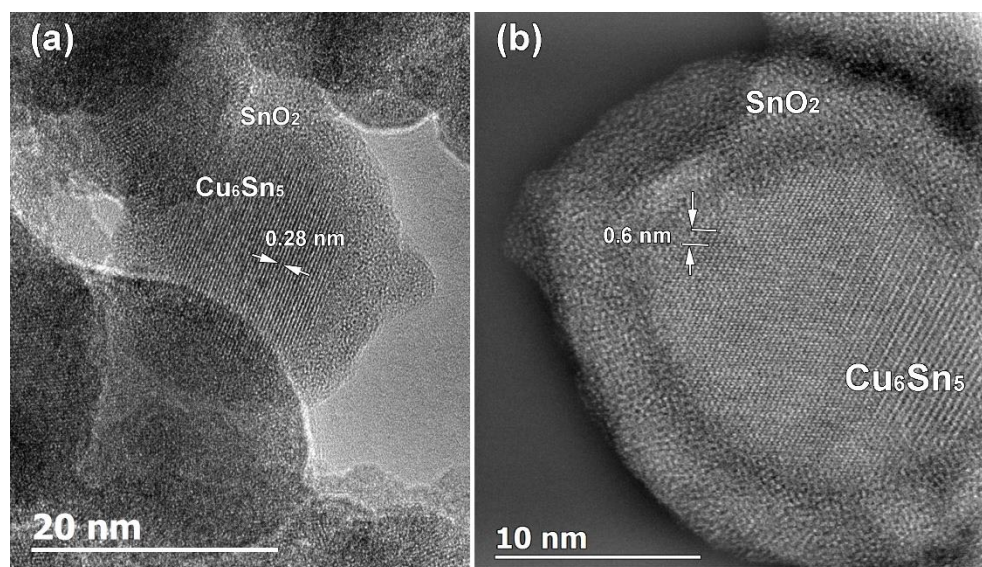


Figure S7. Transmission electron micrographs of Cu-Sn nanoparticles.

Table S1. List of N-H and N-F (highlighted in green) inter-atomic distances as found in the orthorhombic crystal structure of [emim]OTf.^[1] The labels of atoms and their coordinates in the crystallographic cell are taken from the CIF file. The corresponding location of atoms is also given.

	Label	Atoms and location	x	y	z	Distance (Å)
N1	N1	N carrying the ethyl chain in the cation	0.7301	0.7036	0.561	
	H2	H from imidazolium ring	0.8379	0.722	0.5571	2.0019
	H6B	H from CH2 of the ethyl chain	0.7609	0.4895	0.5925	2.0257
	H6A	H from CH2 of the ethyl chain	0.6766	0.5077	0.588	2.0262
	H5	H from imidazolium ring	0.628	0.788	0.5544	2.0282
	H7A	H from CH3 of the ethyl chain	0.6879	0.5079	0.4609	2.6784
	H7C	H from CH3 of the ethyl chain	0.7699	0.4674	0.4699	2.7875
	H4	H from imidazolium ring	0.6827	1.041	0.5552	3.0417
	H7B	H from CH3 of the ethyl chain	0.7107	0.3486	0.4934	3.3467
	H15	H from imidazolium ring	0.6244	0.7179	0.7167	3.5814
	H8A	H from the methyl chain	0.8845	0.9912	0.5447	3.7962
	H8C	H from the methyl chain	0.8309	1.0844	0.4975	3.9701
	F2	F	0.7818	0.8176	0.3634	4.0445
	H8B	H from the methyl chain	0.8348	1.1191	0.5773	4.086
	F3	F	0.6722	0.7527	0.3549	4.1322

	F1	F	0.7013	0.9813	0.3835	4.2075
	H18B	H from the methyl chain	0.8733	0.498	0.7126	4.3225
	H18C	H from the methyl chain	0.931	0.6172	0.686	4.49
	H16B	H from CH2 of the ethyl chain	0.5765	0.9952	0.6907	4.5429
	F11	F	0.5357	0.6955	0.4114	4.6082
	F8	F	0.9412	0.7798	0.4341	4.6532
	H14	H from imidazolium ring	0.5705	0.4654	0.7304	4.8557
	Label	Element and correspondance	x	y	z	Distance (A)
N3	N3	N carrying the methyl chain in the cation	0.7822	0.9241	0.5552	
	H8A	H from the methyl chain	0.8845	0.9912	0.5447	1.9893
	H8B	H from the methyl chain	0.8348	1.1191	0.5773	1.9893
	H8C	H from the methyl chain	0.8309	1.0844	0.4975	1.9895
	H2	H from imidazolium ring	0.8379	0.722	0.5571	2.0254
	H4	H from imidazolium ring	0.6827	1.041	0.5552	2.0988
	H5	H from imidazolium ring	0.628	0.788	0.5544	3.0847
	F1	F	0.7013	0.9813	0.3835	3.6624
	F2	F	0.7818	0.8176	0.3634	3.8057
	H6B	H from CH2 of the ethyl chain	0.7609	0.4895	0.5925	3.8373
	F8	F	0.9412	0.7798	0.4341	3.9545
	H7B	H from CH3 of the ethyl chain	0.7107	1.3486	0.4934	4.0711
	H6A	H from CH2 of the ethyl chain	0.6766	0.5077	0.588	4.1372
	H7C	H from CH3 of the ethyl chain	0.7699	0.4674	0.4699	4.2742
	H7A	H from CH3 of the ethyl chain	0.6879	0.5079	0.4609	4.3851
	H18C	H from the methyl chain	0.931	0.6172	0.686	4.5748
	F12	F	0.9289	1.2373	0.425	4.577
	F3	F	0.6722	0.7527	0.3549	4.6045
	H15	H from imidazolium ring	0.6244	0.7179	0.7167	4.6212
	H16A	H from CH2 of the ethyl chain	0.9927	0.9846	0.6835	4.641
	H16B	H from CH2 of the ethyl chain	0.5765	0.9952	0.6907	4.6544
	H12	H from imidazolium ring	0.9166	1.226	0.7086	4.657
	F7	F	1.013	0.9618	0.4581	4.6723
	F4	F	0.796	1.2728	0.3575	4.8583
	H6B	H from CH2 of the ethyl chain	0.7609	1.4895	0.5925	4.9454

	H7C	H from CH3 of the ethyl chain	0.7699	1.4674	0.4699	4.9712
	Label	Element and correspondance	x	y	z	Distance (A)
N11	N11	N carrying the ethyl chain in the cation	0.0213	0.1967	0.7161	
	H12	H from imidazolium ring	-0.0834	0.226	0.7086	1.9586
	H16A	H from CH2 of the ethyl chain	-0.0073	-0.0154	0.6835	2.0053
	H16B	H from CH2 of the ethyl chain	0.0765	0.0048	0.6907	2.0055
	H15	H from imidazolium ring	0.1244	0.2821	0.7167	2.0446
	H17C	H from CH3 of the ethyl chain	-0.0057	0.0079	0.8093	2.4743
	H17A	H from CH3 of the ethyl chain	0.0752	-0.0428	0.8009	2.8157
	H14	H from imidazolium ring	0.0705	0.5346	0.7304	3.0659
	H17B	H from CH3 of the ethyl chain	0.013	-0.1518	0.7749	3.216
	H5	H from imidazolium ring	0.128	0.212	0.5544	3.6888
	H18B	H from the methyl chain	-0.1267	0.498	0.7126	3.7756
	F9	F	-0.0477	0.2462	0.9021	3.826
	H18A	H from the methyl chain	-0.081	0.5943	0.7659	4.0328
	H18C	H from the methyl chain	-0.069	0.6172	0.686	4.0352
	F8	F	0.0588	0.2202	0.9341	4.2593
	H8B	H from the methyl chain	-0.1652	0.1191	0.5773	4.4152
	F5	F	-0.1869	0.2953	0.8267	4.4825
	F10	F	0.0498	0.5331	0.8924	4.4969
	H8A	H from the methyl chain	-0.1155	-0.0088	0.5447	4.5209
	H6A	H from CH2 of the ethyl chain	0.1766	0.4923	0.588	4.565
	F2	F	0.2182	0.1824	0.8634	4.6181
	H4	H from imidazolium ring	0.1827	-0.041	0.5552	4.7662
	F7	F	-0.013	0.0382	0.9581	4.8974
	Label	Element and correspondance	x	y	z	Distance (A)
N13	N13	N carrying the methyl chain in the cation	0.9731	0.4252	0.7223	
	H18A	H from the methyl chain	0.919	0.5943	0.7659	1.9581
	H18B	H from the methyl chain	0.8733	0.498	0.7126	1.959
	H18C	H from the methyl chain	0.931	0.6172	0.686	1.9591
	H12	H from imidazolium ring	0.9166	0.226	0.7086	2.0284
	H14	H from imidazolium ring	1.0705	0.5346	0.7304	2.0399
	H15	H from imidazolium ring	1.1244	0.2821	0.7167	3.0609
	F10	F	1.0498	0.5331	0.8924	3.6887

	F5	F	0.8131	0.2953	0.8267	3.7493
	F9	F	0.9523	0.2462	0.9021	3.8102
	H17B	H from CH3 of the ethyl chain	1.013	0.8482	0.7749	3.858
	H16A	H from CH2 of the ethyl chain	0.9927	-0.0154	0.6835	3.8903
	H17C	H from CH3 of the ethyl chain	0.9943	0.0079	0.8093	3.9896
	H16B	H from CH2 of the ethyl chain	1.0765	0.0048	0.6907	4.1448
	F11	F	0.9643	0.6955	0.9114	4.3267
	F6	F	0.7385	0.4649	0.7993	4.5989
	H6A	H from CH2 of the ethyl chain	1.1766	0.4923	0.588	4.6037
	H8B	H from the methyl chain	0.8348	0.1191	0.5773	4.6165
	F3	F	0.8278	0.7527	0.8549	4.6609
	H6B	H from CH2 of the ethyl chain	0.7609	0.4895	0.5925	4.6865
	H5	H from imidazolium ring	1.128	0.212	0.5544	4.6952
	H17A	H from CH3 of the ethyl chain	1.0752	-0.0428	0.8009	4.7069
	F8	F	1.0588	0.2202	0.9341	4.7193
	H2	H from imidazolium ring	0.8379	0.722	0.5571	4.7883
	H16A	H from CH2 of the ethyl chain	0.9927	0.9846	0.6835	4.8963
	Label	Element and correspondance	x	y	z	Distance (A)
N14	N14	N of the anion	0.7204	0.0393	0.7455	
	H16B	H from imidazolium ring	0.5765	-0.0048	0.6907	2.8887
	H17A	H from CH3 of the ethyl chain	0.5752	0.0428	0.8009	2.8903
	F4	F	0.704	0.2728	0.8575	2.9664
	F2	F	0.7182	-0.1824	0.8634	2.9686
	F1	F	0.7987	-0.0187	0.8835	3.0674
	F5	F	0.8131	0.2953	0.8267	3.2034
	H15	H from imidazolium ring	0.6244	-0.2821	0.7167	3.3388
	H4	H from imidazolium ring	0.6827	0.041	0.5552	3.73
	F3	F	0.8278	-0.2473	0.8549	3.8074
	F6	F	0.7385	0.4649	0.7993	3.8292
	H8B	H from the methyl chain	0.8348	0.1191	0.5773	3.9296
	H17B	H from CH3 of the ethyl chain	0.513	0.1518	0.7749	3.9978
	H12	H from imidazolium ring	0.9166	0.226	0.7086	4.0338
	H17C	H from CH3 of the ethyl chain	0.4943	-0.0079	0.8093	4.3783

	H16A	H from CH2 of the ethyl chain	0.4927	0.0154	0.6835	4.383
	H5	H from imidazolium ring	0.628	-0.212	0.5544	4.6
	H14	H from imidazolium ring	0.5705	0.4654	0.7304	4.6134
	F12	F	0.5711	0.2373	0.925	4.7425
	H18B	H from the methyl chain	0.8733	0.498	0.7126	4.9048
	H6B	H from CH2 of the ethyl chain	0.7609	0.4895	0.5925	4.9316
	H8A	H from the methyl chain	0.8845	-0.0088	0.5447	4.9332
	H8C	H from the methyl chain	0.6691	0.0844	0.9975	4.9595
	Label	Element and correspondance	x	y	z	Distance (A)
N15	N	N of the anion	0.9655	0.4597	0.0213	
	F11	F	0.9643	0.6955	-0.0886	2.9352
	F9	F	0.9523	0.2462	-0.0979	2.9528
	H6A	H from CH2 of the ethyl chain	0.8234	0.5077	0.088	2.9548
	F10	F	1.0498	0.5331	-0.1076	2.9988
	H7A	H from CH3 of the ethyl chain	0.8121	0.5079	-0.0391	3.0949
	F8	F	1.0588	0.2202	-0.0659	3.1727
	H5	H from imidazolium ring	0.872	0.788	0.0544	3.379
	H7B	H from CH3 of the ethyl chain	0.7893	0.3486	-0.0066	3.4397
	F12	F	1.0711	0.7627	-0.075	3.7531
	H18C	H from the methyl chain	1.069	0.3828	0.186	3.7634
	F7	F	0.987	0.0382	-0.0419	3.8547
	H2	H from imidazolium ring	1.1621	0.278	0.0571	4.0198
	H14	H from imidazolium ring	0.9295	0.4654	0.2304	4.0812
	H6B	H from CH2 of the ethyl chain	0.7391	0.4895	0.0925	4.4143
	H7C	H from CH3 of the ethyl chain	0.7301	0.4674	-0.0301	4.4662
	H4	H from imidazolium ring	0.8173	0.041	0.0552	4.5811
	H15	H from imidazolium ring	0.8756	0.7179	0.2167	4.6778
	H18B	H from the methyl chain	1.1267	0.502	0.2126	4.7533
	H8A	H from the methyl chain	1.1155	0.0088	0.0447	4.799
	F3	F	0.8278	0.7527	-0.1451	4.8106
	F5	F	0.8131	0.2953	-0.1733	4.8989

Table S2. Calculation of the theoretical and rescaled capacities.

Phases	Theoretical capacity with and without(/) conversion process (mAh.g⁻¹)	Proportions (%)	Rescaled capacity (mAh.g⁻¹)
Cu ₆ Sn _{3.3} □ _{1.75}	503	51	256.5
SnO	1274/874	10	127.4/87.4
SnO ₂	1494/781	39	582.6/304.6
Total			966.5/648.5

[1] A. R. Choudhury, N. Winterton, A. Steiner, A. I. Cooper, K. A. Johnson, *CrystEngComm* **2006**, *8*, 742–745.