

Realising higher capacity and stability for disordered rocksalt oxyfluoride cathode materials for Li ion batteries

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Table S1: Results from ICP-AES for LMTOF.

Element	LMTO 5% excess in Li ₂ CO ₃		
	Li4602	Mn2576	Ti3349
Unit	ppm	ppm	ppm
Avg	8.723	23.03	20.07
Stddev	0.03	0.04	0.08
%RSD	0.2913	0.192	0.3895

Table S2: Results from ICP-AES for LMTOF.

Element	LMTOF 20% excess in Li ₂ CO ₃		
	Li4602	Mn2576	Ti3349
Unit	ppm	ppm	ppm
Avg	3.028	8.011	4.715
Stddev	0.054	0.019	0.039
%RSD	1.79	0.2336	0.8249

Table S3: Rietveld refinement for LMTO and LMTOF materials.

Materials	Atom	Site	X	Y	Z	fraction	Rwp	GOF (good of fitness)
Li _{1.2} Mn _{0.4} Ti _{0.4} O ₂	Li	4a	0	0	0	0.6	0.0377	1.91
	Mn	4a	0	0	0	0.2		
	Ti	4a	0	0	0	0.2		
	O	4b	1/2	1/2	1/2	1		
Li _{1.2} Mn _{0.4} Ti _{0.3} O _{1.7} F _{0.3}	Li	4a	0	0	0	0.6	0.0535	2.27
	Mn	4a	0	0	0	0.2		
	Ti	4a	0	0	0	0.15		
	O	4b	1/2	1/2	1/2	0.85		
	F	4b	1/2	1/2	1/2	0.15		

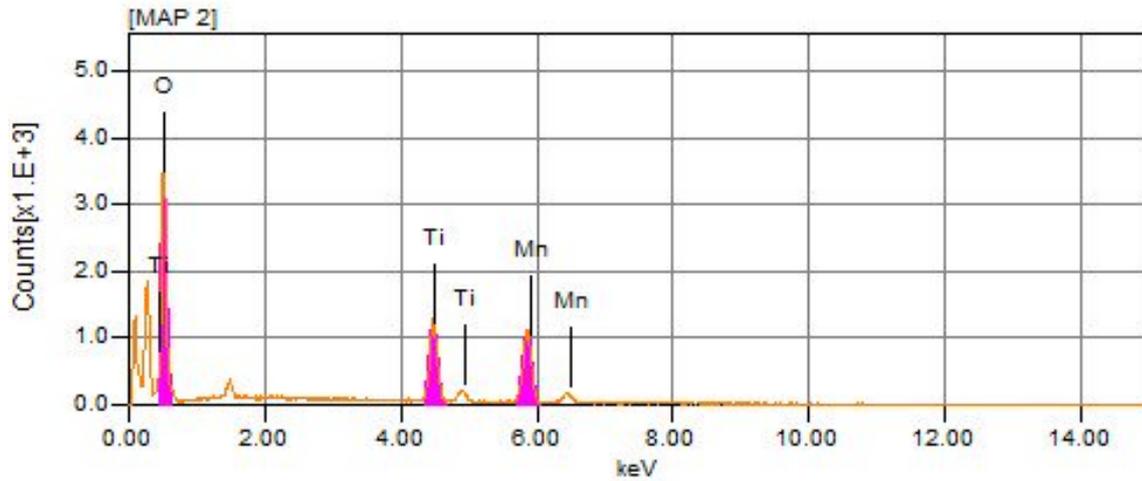


Figure S1: EDS spectrum for the EDS elemental mapping of the SEM image of LMTOF@C, showing the presence of Ti and Mn.

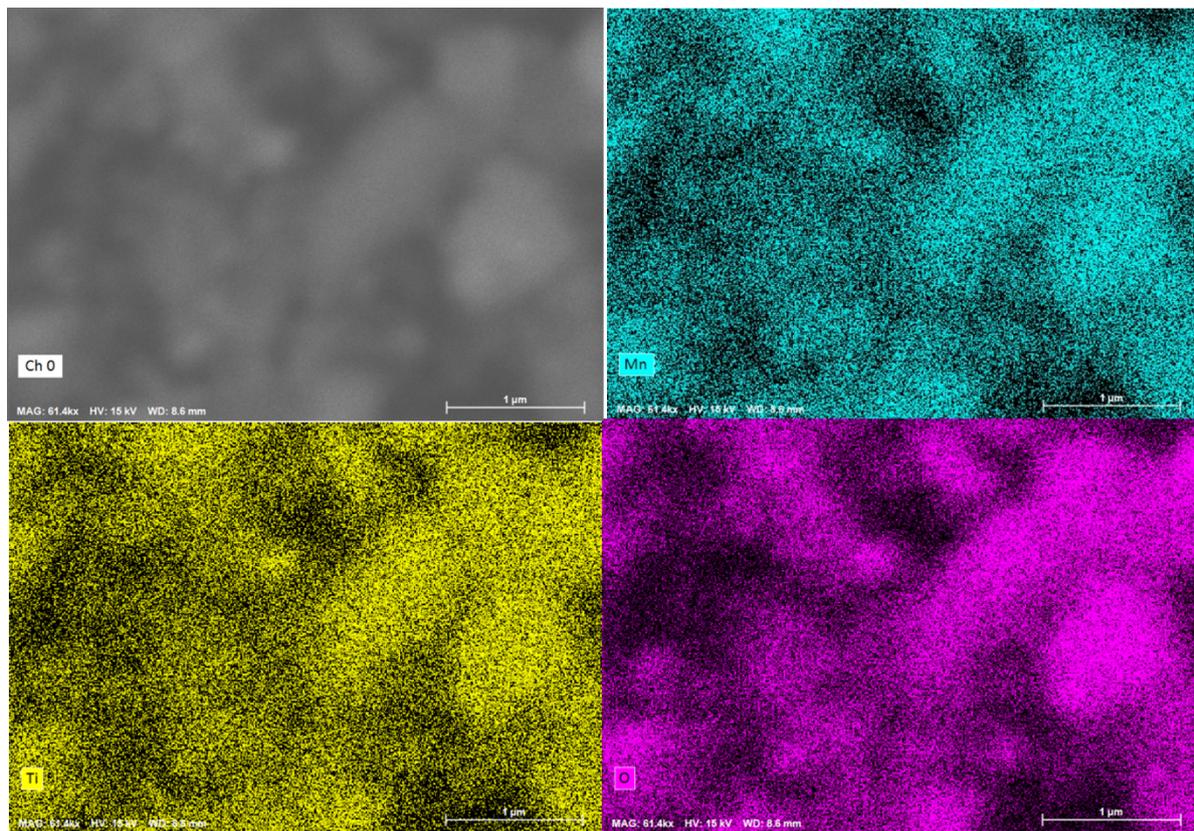


Figure S2: SEM image of LMTO@C and the corresponding EDS mapping of Mn, Ti and O.

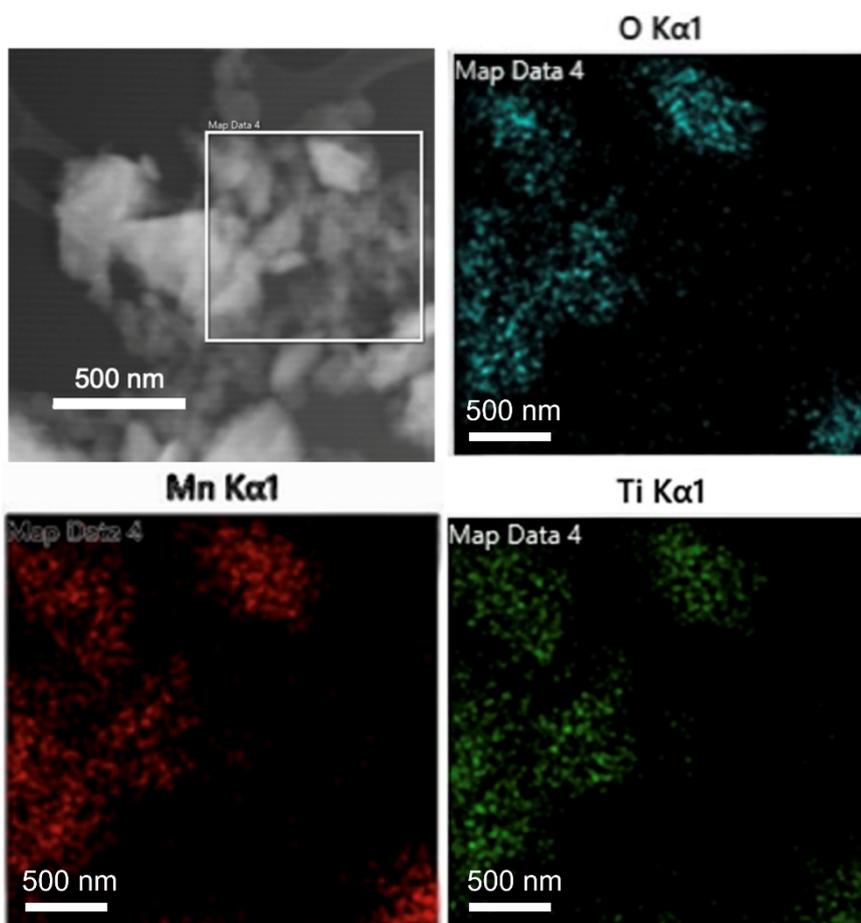


Figure S3: TEM image of individual particles of LMTO@C and the corresponding EDS mapping of the particles.

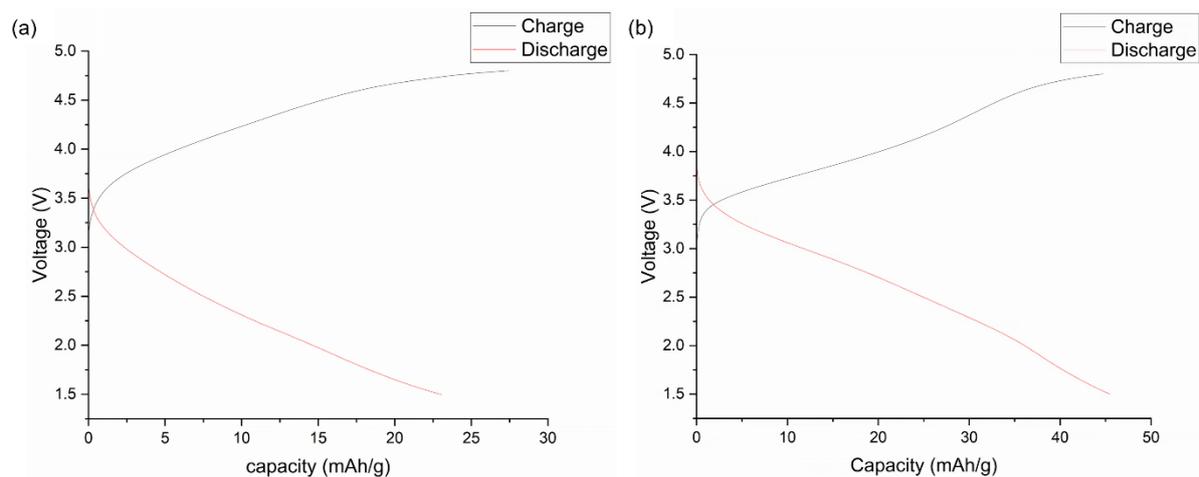


Figure S4: charging and discharge curve of LMTO-B, LMTOF-B between 1.5-4.8 V at 0.5 C.

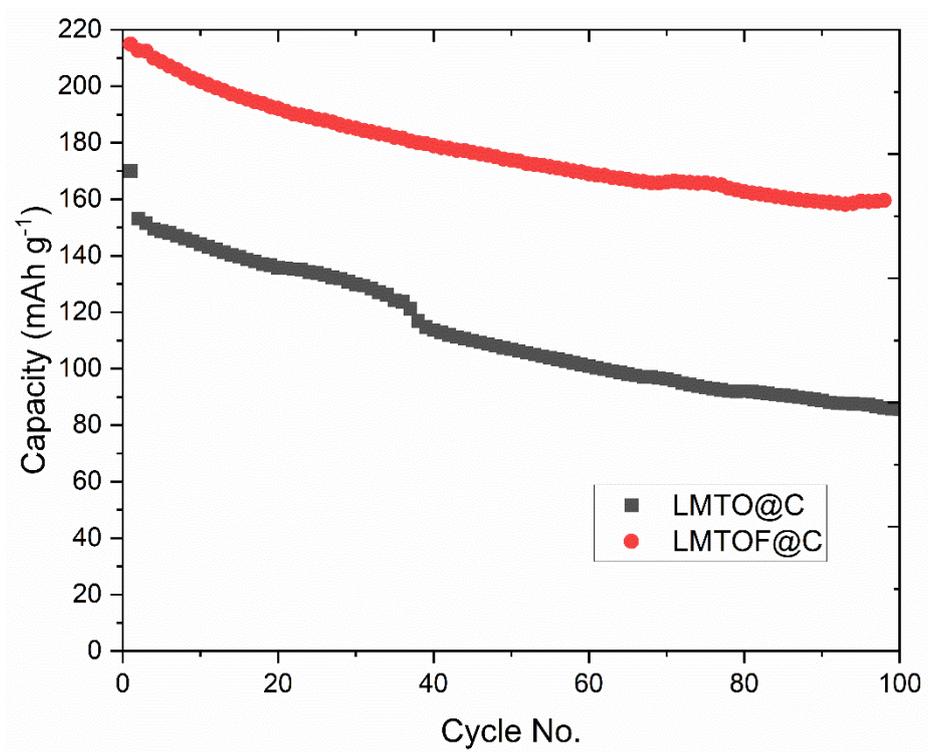


Figure S5: Cycling performance of LMTO@C, LMTOF@C between 1.5-4.8 V at 0.5 C.