Supplementary information

Fig. S1 : Definition of the blocks used to simulate the presence of spinel-type domains in the Li_2MnO_3 stacking

The two structures are described using the same unit cell (a = 10.10 Å, b = 17.50 Å). Concerning the Li_2MnO_3 stacking, the thickness of the slab is 2.14 Å and that of the interslabr is 2.61 Å. Concerning the $LiMn_2O_4$ stacking, the thickness of the slab is 2.17 Å and that of the interslab is 2.59 Å.

Description the Li_2MnO_3 cell

Atom	x	y	z	Occ. fact	B_{iso}
O	0.0	0.0	0.0	1.0	1.0
O	1/2	0.0	0.0	1.0	1.0
O	1/4	1/12	0.0	1.0	1.0
O	3/4	1/12	0.0	1.0	1.0
O	0.0	1/6	0.0	1.0	1.0
O	1/2	1/6	0.0	1.0	1.0
O	1/4	1/4	0.0	1.0	1.0
O	3/4	1/4	0.0	1.0	1.0
O	0.0	1/3	0.0	1.0	1.0
O	1/2	1/3	0.0	1.0	1.0
O	1/4	5/12	0.0	1.0	1.0
O	3/4	5/12	0.0	1.0	1.0
O	0.0	1/2	0.0	1.0	1.0
O	1/2	1/2	0.0	1.0	1.0
O	1/4	7/12	0.0	1.0	1.0
O	3/4	7/12	0.0	1.0	1.0
O	0.0	2/3	0.0	1.0	1.0
O	1/2	2/3	0.0	1.0	1.0
O	1/4	3/4	0.0	1.0	1.0
O	3/4	3/4	0.0	1.0	1.0
O	0.0	5/6	0.0	1.0	1.0
O	1/2	5/6	0.0	1.0	1.0
O	1/4	11/12	0.0	1.0	1.0
O	3/4	11/12	0.0	1.0	1.0
Mn	1/3	1/6	0.225	1.0	1.0
Mn	5/6	1/6	0.225	1.0	1.0
Mn	1/12	1/4	0.225	1.0	1.0
Mn	7/12	1/4	0.225	1.0	1.0
Mn	1/12	5/12	0.225	1.0	1.0
Mn	7/12	5/12	0.225	1.0	1.0
Mn	1/3	1/2	0.225	1.0	1.0
Mn	5/6	1/2	0.225	1.0	1.0
Mn	1/3	2/3	0.225	1.0	1.0
Mn	5/6	2/3	0.225	1.0	1.0
Mn	1/12	3/4	0.225	1.0	1.0
Mn	7/12	3/4	0.225	1.0	1.0
Mn	1/12	11/12	0.225	1.0	1.0
Mn	7/12	11/12	0.225	1.0	1.0
Mn	1/3	1.0	0.225	1.0	1.0

Mn	5/6	1.0	0.225	1.0	1.0
Li	1/12	1/12	0.225	1.0	1.0
Li	7/12	1/12	0.225	1.0	1.0
Li	1/3	1/3	0.225	1.0	1.0
Li	5/6	1/3	0.225	1.0	1.0
Li	1/12	7/12	0.225	1.0	1.0
Li	7/12	7/12	0.225	1.0	1.0
Li	1/3	5/6	0.225	1.0	1.0
Li	5/6	5/6	0.225	1.0	1.0
O	1/6	0.0	0.45	1.0	1.0
O	2/3	0.0	0.45	1.0	1.0
O	5/12	1/12	0.45	1.0	1.0
O	11/12	1/12	0.45	1.0	1.0
O	1/6	1/6	0.45	1.0	1.0
O	2/3	1/6	0.45	1.0	1.0
O	5/12	1/4	0.45	1.0	1.0
O	11/12	1/4	0.45	1.0	1.0
O	1/6	1/3	0.45	1.0	1.0
O	2/3	1/3	0.45	1.0	1.0
O	5/12	5/12	0.45	1.0	1.0
O	11/12	5/12	0.45	1.0	1.0
O	1/6	1/2	0.45	1.0	1.0
O	2/3	1/2	0.45	1.0	1.0
O	5/12	7/12	0.45	1.0	1.0
O	11/12	7/12	0.45	1.0	1.0
O	1/6	2/3	0.45	1.0	1.0
O	2/3	2/3	0.45	1.0	1.0
O	5/12	3/4	0.45	1.0	1.0
O	11/12	3/4	0.45	1.0	1.0
O	1/6	5/6	0.45	1.0	1.0
O	2/3	5/6	0.45	1.0	1.0
O	5/12	11/12	0.45	1.0	1.0
O	11/12	11/12	0.45	1.0	1.0
Li	1/2	1/6	0.777	1.0	1.0
Li	1.0	1/6	0.777	1.0	1.0
Li	1/4	1/4	0.777	1.0	1.0
Li	3/4	1/4	0.777	1.0	1.0
Li	1/4	5/12	0.777	1.0	1.0
Li	3/4	5/12	0.777	1.0	1.0
Li	1/2	1/2	0.777	1.0	1.0
Li	1.0	1/2	0.777	1.0	1.0
Li	1/2	2/3	0.777	1.0	1.0
Li	1.0	2/3	0.777	1.0	1.0
Li	1/4	3/4	0.777	1.0	1.0
Li	3/4	3/4	0.777	1.0	1.0
Li	1/4	11/12	0.777	1.0	1.0
Li	3/4	11/12	0.777	1.0	1.0
Li	1/2	1.0	0.777	1.0	1.0
Li	1.0	1.0	0.777	1.0	1.0
Li	1/4	1/12	0.777	1.0	1.0
Li	3/4	1/12	0.777	1.0	1.0
Li	1/2	1/3	0.777	1.0	1.0
Li	1.0	1/3	0.777	1.0	1.0
Li	1/4	7/12	0.777	1.0	1.0
Li	3/4	7/12	0.777	1.0	1.0
Li	1/2	5/6	0.777	1.0	1.0
Li	1.0	5/6	0.777	1.0	1.0

Description the $LiMn_2O_4$ cell

Atom	x	y	z	Occ. fact	B_{iso}
O	0.0	0.0	0.0	1.0	1.0
O	1/2	0.0	0.0	1.0	1.0
O	1/4	1/12	0.0	1.0	1.0
O	3/4	1/12	0.0	1.0	1.0
O	0.0	1/6	0.0	1.0	1.0
O	1/2	1/6	0.0	1.0	1.0
O	1/4	1/4	0.0	1.0	1.0
O	3/4	1/4	0.0	1.0	1.0
O	0.0	1/3	0.0	1.0	1.0
O	1/2	1/3	0.0	1.0	1.0
O	1/4	5/12	0.0	1.0	1.0
O	3/4	5/12	0.0	1.0	1.0
O	0.0	1/2	0.0	1.0	1.0
O	1/2	1/2	0.0	1.0	1.0
O	1/4	7/12	0.0	1.0	1.0
O	3/4	7/12	0.0	1.0	1.0
O	0.0	2/3	0.0	1.0	1.0
O	1/2	2/3	0.0	1.0	1.0
O	1/4	3/4	0.0	1.0	1.0
O	3/4	3/4	0.0	1.0	1.0
O	0.0	5/6	0.0	1.0	1.0
O	1/2	5/6	0.0	1.0	1.0
O	1/4	11/12	0.0	1.0	1.0
O	3/4	11/12	0.0	1.0	1.0
Mn	1/12	1/12	0.231	1.0	1.0
Mn	7/12	1/12	0.231	1.0	1.0
Mn	1/3	1/6	0.231	1.0	1.0
Mn	1/12	1/4	0.231	1.0	1.0
Mn	7/12	1/4	0.231	1.0	1.0
Mn	5/6	1/3	0.231	1.0	1.0
Mn	1/12	5/12	0.231	1.0	1.0
Mn	7/12	5/12	0.231	1.0	1.0
Mn	1/3	1/2	0.231	1.0	1.0
Mn	1/12	7/12	0.231	1.0	1.0
Mn	7/12	7/12	0.231	1.0	1.0
Mn	5/6	2/3	0.231	1.0	1.0
Mn	1/12	3/4	0.231	1.0	1.0
Mn	7/12	3/4	0.231	1.0	1.0
Mn	1/3	5/6	0.231	1.0	1.0
Mn	1/12	11/12	0.231	1.0	1.0
Mn	7/12	11/12	0.231	1.0	1.0
Mn	5/6	1	0.231	1.0	1.0
O	1/6	0	0.462	1.0	1.0
O	2/3	0	0.462	1.0	1.0
O	5/12	1/12	0.462	1.0	1.0
O	11/12	1/12	0.462	1.0	1.0
O	1/6	1/6	0.462	1.0	1.0
O	2/3	1/6	0.462	1.0	1.0
O	5/12	1/4	0.462	1.0	1.0
O	11/12	1/4	0.462	1.0	1.0
O	1/6	1/3	0.462	1.0	1.0
O	2/3	1/3	0.462	1.0	1.0
O	5/12	5/12	0.462	1.0	1.0
O	11/12	5/12	0.462	1.0	1.0
O	1/6	1/2	0.462	1.0	1.0
O	2/3	1/2	0.462	1.0	1.0
O	5/12	7/12	0.462	1.0	1.0
O	11/12	7/12	0.462	1.0	1.0
O	1/6	2/3	0.462	1.0	1.0
O	2/3	2/3	0.462	1.0	1.0

O	5/12	3/4	0.462	1.0	1.0
O	11/12	3/4	0.462	1.0	1.0
O	1/6	5/6	0.462	1.0	1.0
O	2/3	5/6	0.462	1.0	1.0
O	5/12	11/12	0.462	1.0	1.0
O	11/12	11/12	0.462	1.0	1.0
Li	2/3	0.0	0.866	1.0	1.0
Li	1/6	1/6	0.866	1.0	1.0
Li	2/3	1/3	0.866	1.0	1.0
Li	1/6	1/2	0.866	1.0	1.0
Li	2/3	2/3	0.866	1.0	1.0
Li	1/6	5/6	0.866	1.0	1.0
Li	1/3	0.0	0.597	1.0	1.0
Li	5/6	1/6	0.597	1.0	1.0
Li	1/3	1/3	0.597	1.0	1.0
Li	5/6	1/2	0.597	1.0	1.0
Li	1/3	2/3	0.597	1.0	1.0
Li	5/6	5/6	0.597	1.0	1.0
Mn	0.0	0.0	0.731	1.0	1.0
Mn	1/2	1/6	0.731	1.0	1.0
Mn	0.0	1/3	0.731	1.0	1.0
Mn	1/2	1/2	0.731	1.0	1.0
Mn	0.0	2/3	0.731	1.0	1.0
Mn	1/2	5/6	0.731	1.0	1.0

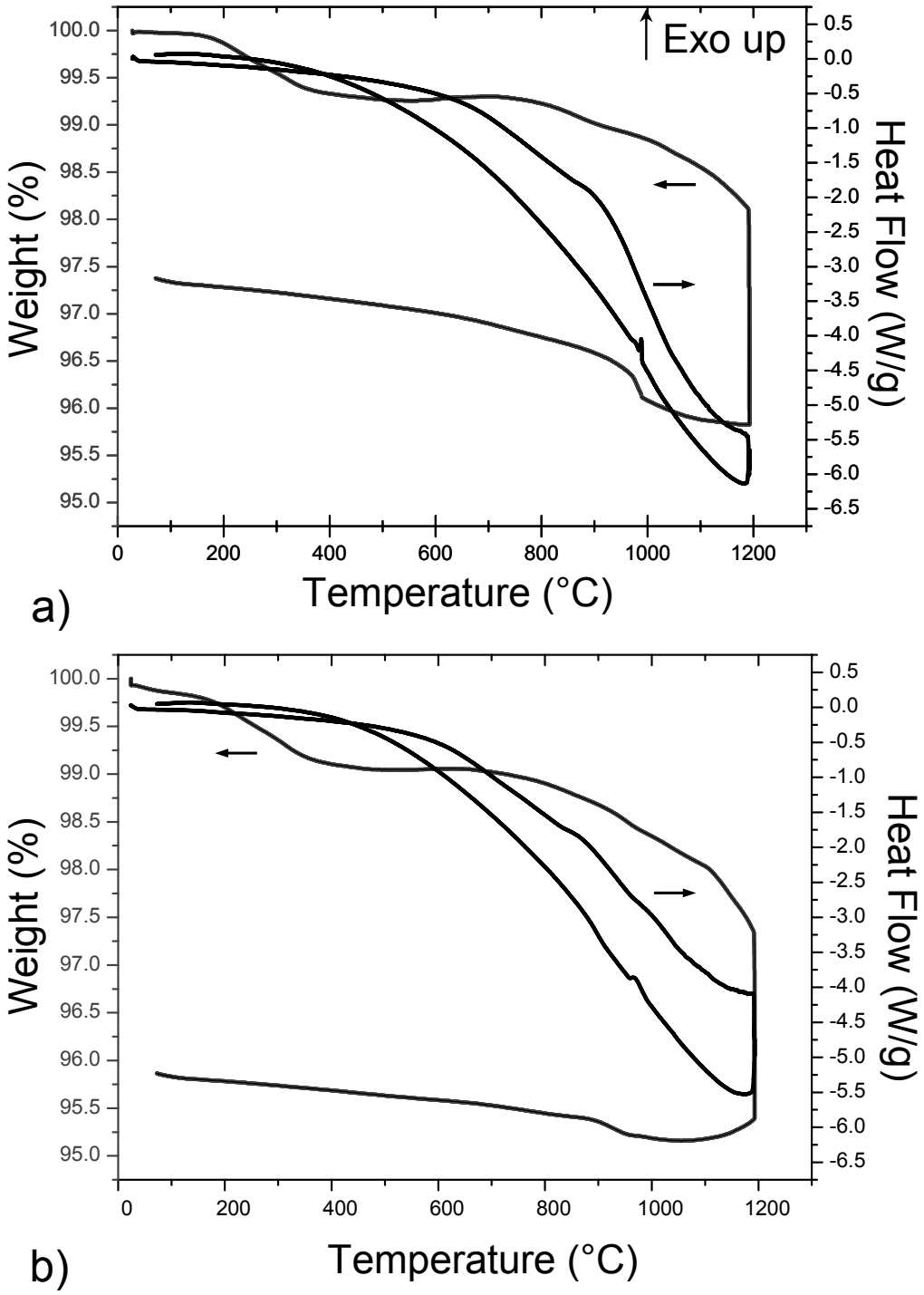

Fig. S2. TGA and DTA curves obtained with the materials recovered after heating the 650°C synthesized powder sample until a) 1200°C in oxygen for 4h and b) 1200°C in argon atmosphere for 1h.