Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Role of Transitions Metals in Charge Transfer Mechanism and Oxygen Evolution in $Li_{1.17}Ni_{0.17}Mn_{0.5}Co_{0.17}O_2$: Experimental and First-Principle Analysis

Tanmay Sarkar,[¥,†,‡] Kunkanadu R. Prakasha,[†,‡] Mridula Dixit Bharadwaj,[¥] Annigere S. Prakash[†,*]

[¥]Center for Study of Science, Technology and Policy (CSTEP), Bangalore 560094, India.

[†]CSIR – Network Institutes of Solar Energy (CSIR – NISE), CSIR – Central Electrochemical Research Institute-Chennai Unit, CSIR Madras Complex, Taramani, Chennai 600113, India.

[‡]Academy of Scientific and Innovative Research (AcSIR), CSIR – Central Electrochemical Research Institute-Chennai Unit, CSIR Madras Complex, Taramani, Chennai 600113, India.

Table S1. Structural parameters obtained from Rietveld refinement of XRD data for Li_2MnO_3 phases with monoclinic (C2/m) symmetry.

Li_2MnO_3					
Space group : C2/m					
Element	Site	Wyckoff positions			Occupancy
Li	4g	0	0.5	0	0.4315
Mn	4g	0	0.5	0	0.4372
Li	4g	0	0	0.5	0.999
Li	2b	0	0.5783	0.5	0.9713
Li	2b	0	0.1660	0	0.4885
Mn	2b	0	0.1660	0	0.6057
O	2c	0.2785	0	0.2068	1.1628
O	4h	0.2364	0.3479	0.2374	1.7452
a = 4.927841 Å, b = 8.528829 Å, c = 5.022231 Å, β = 109.2°					

Table S2. Structural parameters obtained from two phase Rietveld refinement of XRD data for $Li_{1.17}Ni_{0.17}Mn_{0.5}Co_{0.17}O_2$ material.

Pristine $Li_{1.17}Ni_{0.17}Mn_{0.5}Co_{0.17}O_2$					
Phase 1: $LiNi_{1/3}Mn_{1/3}Co_{1/3}O_2$ ($R\bar{3}m$)					
Element	Site	Wyckoff positions			Occupancy
Li1	3b	0	0	0	0.9760
Ni1	3b	0	0	0	0.0241
Li2	3a	0	0	0.5	0.0200
Ni2	3a	0	0	0.5	0.3100
Mn1	3a	0	0	0.5	0.3350
Co1	3a	0	0	0.5	0.3366
O1	6c	0	0	0.2440	1.0000
a = 2.8487A° c = 14.2216A°					
Phase 2: Li_2MnO_3 (C2/m)					
Element	Site	Wyckoff positions			Occupancy
Li1	2b	0	0.5	0	0.8516
Mn1	2b	0	0.5	0	0.1261
Li2	2c	0	0	0.5	1.0080
Li3	4h	0	0.7149	0.5	1.1811
Mn2	4h	0	0.6740	0.5	0.0286
Li4	4g	0	0.0870	0	0.0840
Mn3	4g	0	0.1795	0	0.8507
O1	6c	0.2458	0	0.2130	1.0600
O2	8j	0.2491	0.3281	0.2429	2.0000
a = 4.9540A° b = 8.5153A° c = 5.0094A° β = 108.88°					
Rwp = 10.2 Rp = 15.6 Chi 2 = 2.26					

Formation energy of Conf 5, Conf 6 and Con 7 is -23.43, -23.40 and -23.36 eV/f.u respectively.

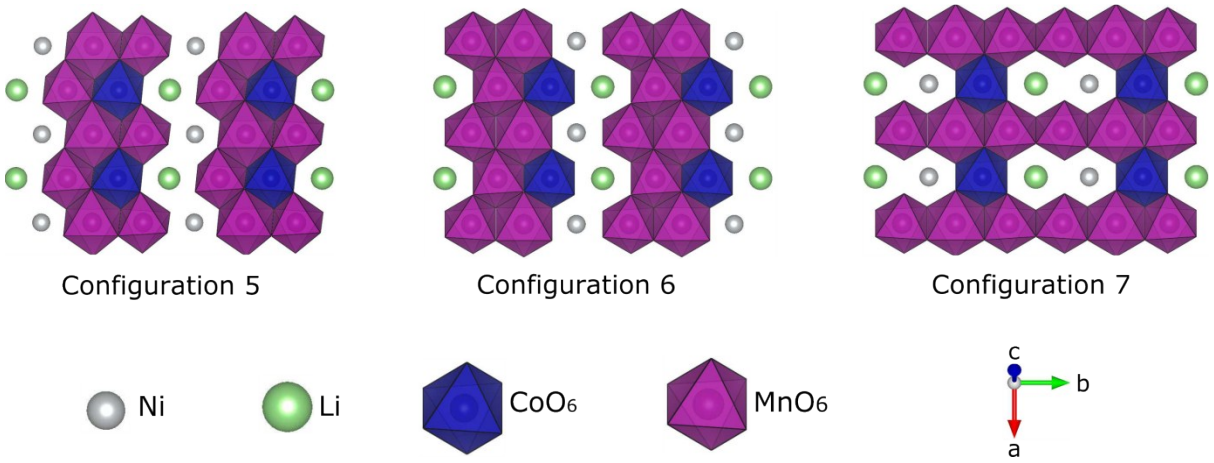

Figure S1: (a) Possible atomic arrangements of 3d metals in LiM_2layer showing different configurations of $Li_{1.17}Ni_{0.17}Mn_{0.5}Co_{0.17}O_2$.

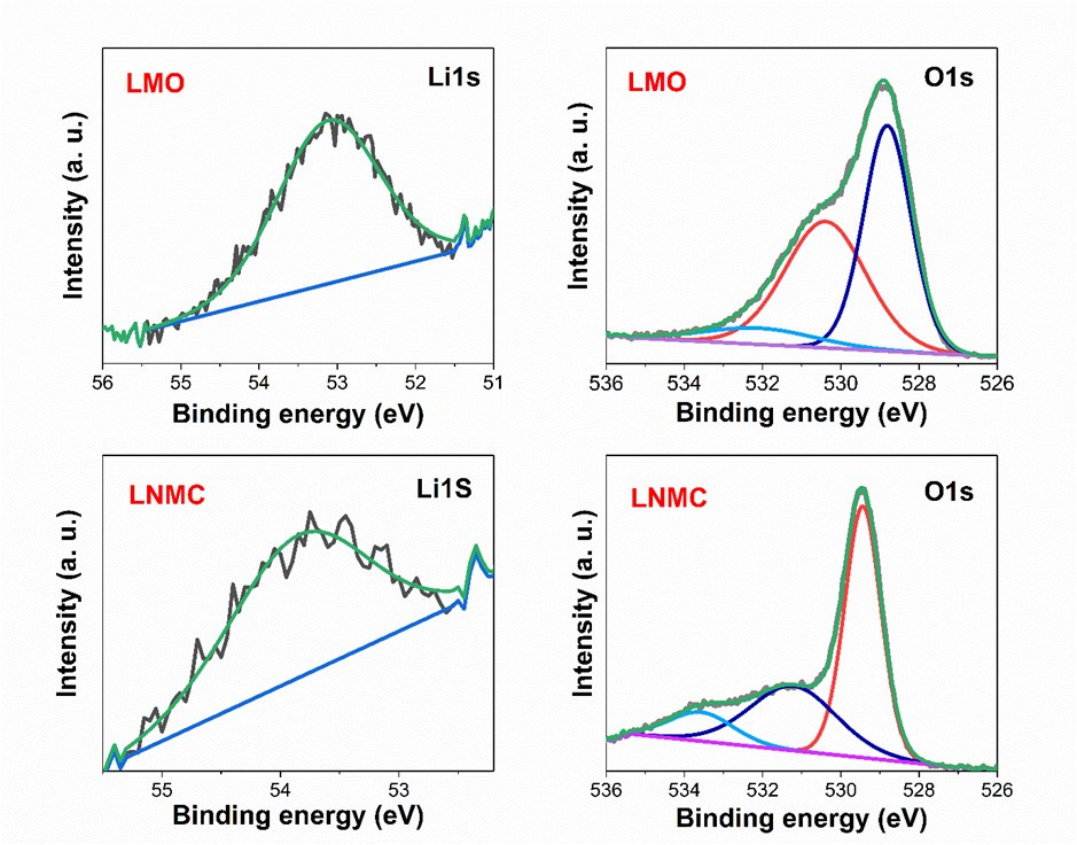

Figure S2: Core level XPS spectra of Li 1s and O 1s peaks for both LMO and LNMC samples.