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Detailed Redox Mechanism and Self-Discharge Diagnostic of 4.9 V $LiMn_{1.5}Ni_{0.5}O_4$ Spinel Cathode revealed by Raman Spectroscopy

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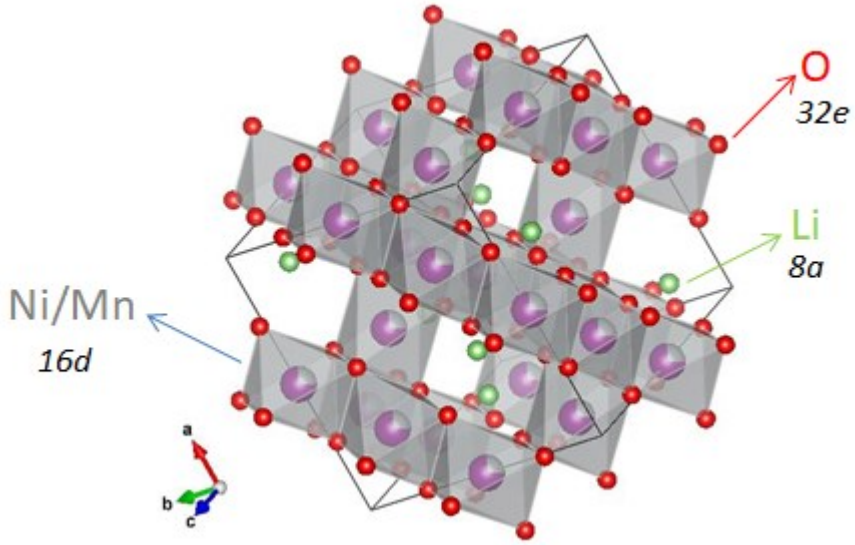
Figure S1. Structure of spinel *Fd3̄m* LMNO (Ni/Mn, O and Li atoms are shown in grey, red and green colour respectively).

Figure S2. XRD pattern of LMNO in the 42-54° 2θ region. Bragg lines marked by green star correspond to impurity peaks. Experimental data shown in red line and calculated pattern in black solid line.

Figure S3. Expected evolution of the Ni^{2+}, Ni^{3+} and Ni^{4+} ratio (indicated by blue, green and red dashed lines, respectively). Estimated $Ni^{2+}/Ni^{3+}/Ni^{4+}$ relative amounts as a function of x in $L_{1-x}NMO$ electrodes obtained from Raman spectra fittings (indicated by blue circles, green squares and red diamonds, respectively). The error bars correspond to statistical error of the deconvolution procedure.

Table S1. Structural parameters obtained from Rietveld refinement of LMNO diffraction pattern



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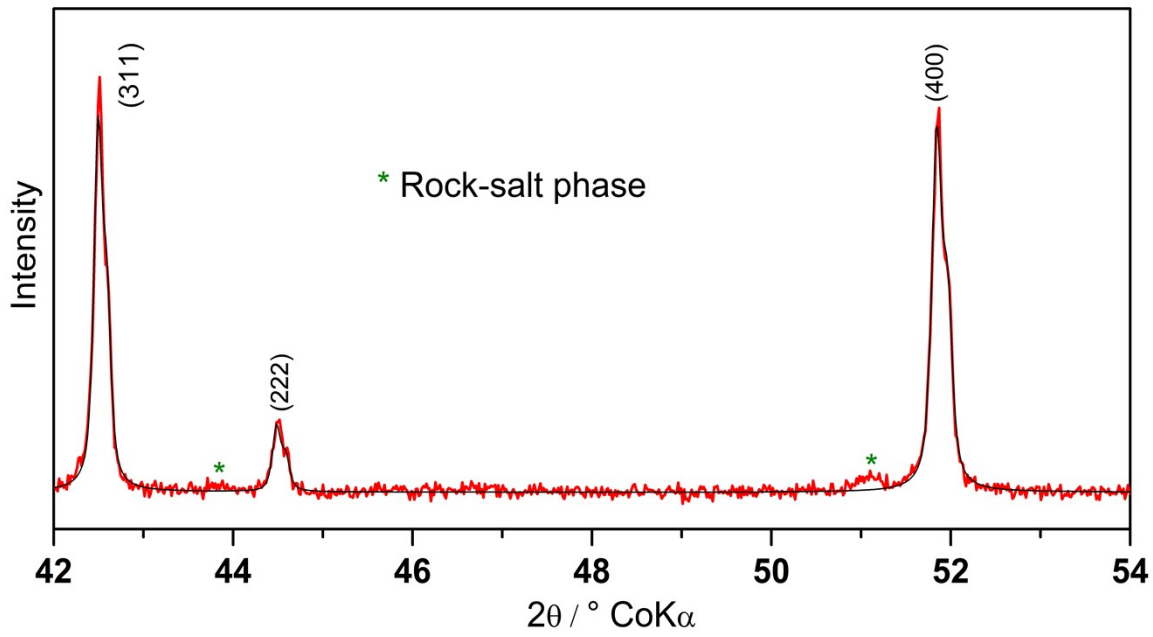

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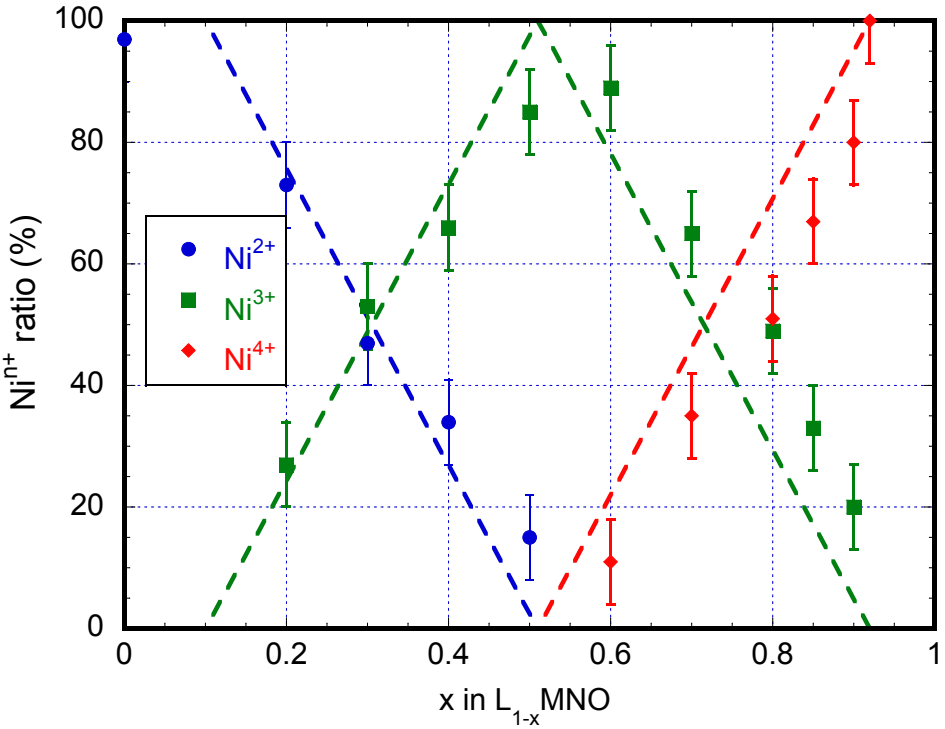

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Atom	Wyckoff position	x	y	z
		Fractional Coordinates		
Li	8a	0.125	0.125	0.125
Ni	16d	0.5	0.5	0.5
Mn	16d	0.5	0.5	0.5
O	32e	0.2600	0.2600	0.2600

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