Structural evolution and high voltage structural stability of $Li(Ni_xMn_yCo_z)O_2$ electrodes

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Supporting information

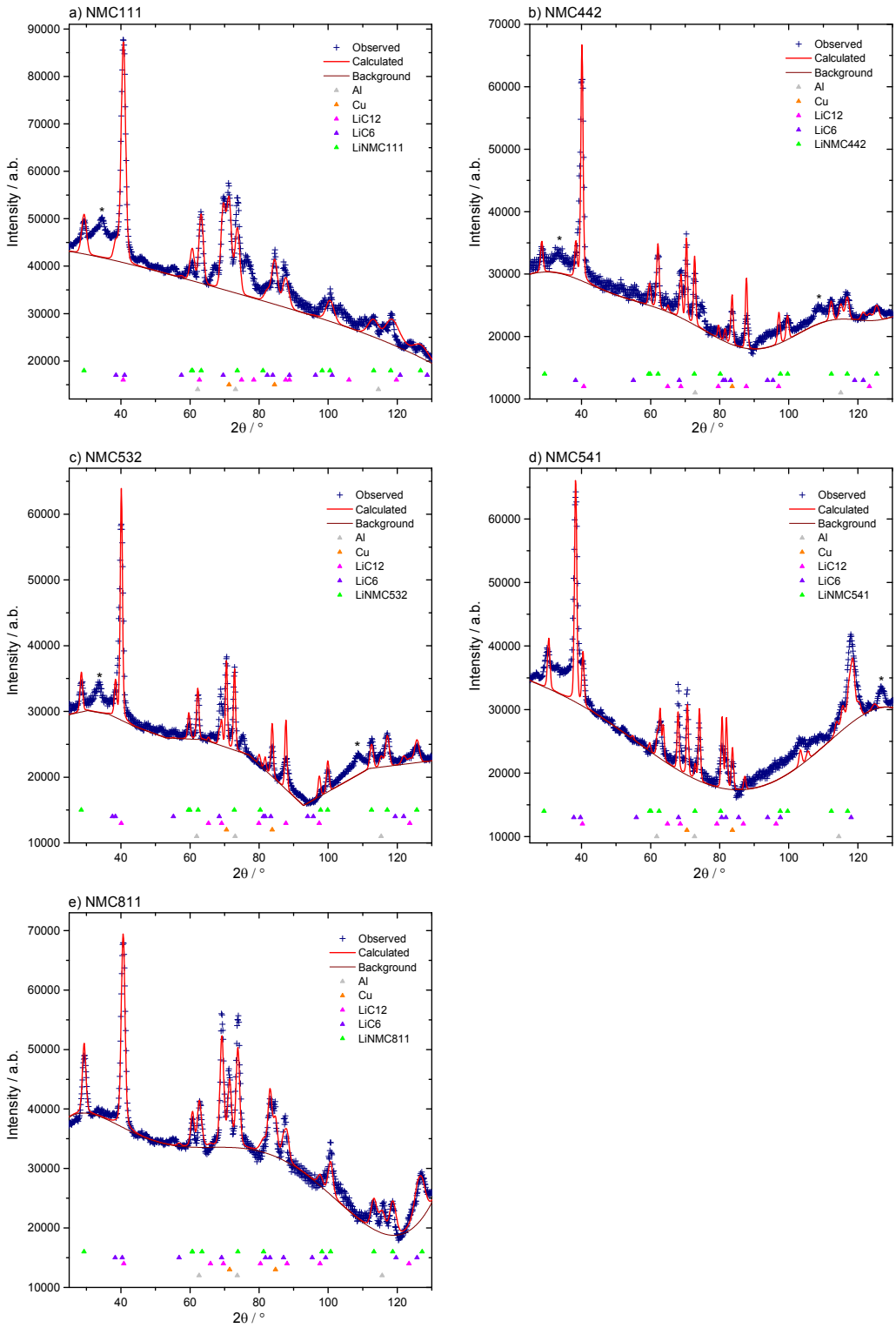

Figure S1 Rietveld refinements profiles of the 1st in-situ neutron diffraction dataset of batteries containing a) NMC111 b) NMC442 c) NMC532 d) NMC541 e) NMC811. Reflections marked with * are contributions from the cell casing which are not electrochemically active.

Table S1 Associated figures of merit for the Rietveld-refined models shown in Figure S1.

	R_w (%)	R (%)	G.O.F	Observations	Bkg. Terms
NMC111	6.31	4.80	12.35	849	5
NMC442	6.23	4.93	10.13	946	11
NMC532	4.79	3.70	7.72	940	11
NMC541	3.50	2.58	5.77	776	10
NMC811	3.98	3.08	7.37	901	7

Table S2 Results of fitting an exponential decay function to the *c* lattice parameter as a function of time during the voltage hold region, see Figure 7.

Equation		y = A1*exp(-x/t1) + y0					
	y0	x0 (t = 0)	A1	t1	Reduced Chi-Sqr	R-Square(COD)	Adj. R-Square
NMC111	13.81413 ± 6.08064E-4	1395 ± 0	0.1055 ± 0.00291	16.25267 ± 0.95797	0.04304	0.96625	0.96502
NMC442	13.99255 ± 4.51343E-4	1150 ± 0	0.08513 ± --	137.13938 ± 3.8948	0.04496	0.98172	0.98155
NMC532	13.88569 ± 5.34349E-4	1233 ± 0	0.07364 ± 0.00139	86.78107 ± 3.35352	0.04067	0.9554	0.95486
NMC541	13.92801 ± 8.60943E-4	1415 ± 0	0.15833 ± 0.00204	43.37615 ± 1.18866	0.10244	0.9932	0.99292
NMC811	13.70873 ± 4.70477E-4	1195 ± 0	0.46998 ± 0.00595	27.18278 ± 0.53533	0.16987	0.98651	0.98638