

A study of room-temperature $\text{Li}_x\text{Mn}_{1.5}\text{Ni}_{0.5}\text{O}_4$ solid solutions

Kuppan Saravanan, Angelique Jarry, Robert Kostecki, and Guoying Chen

Environmental Energy Technologies Division

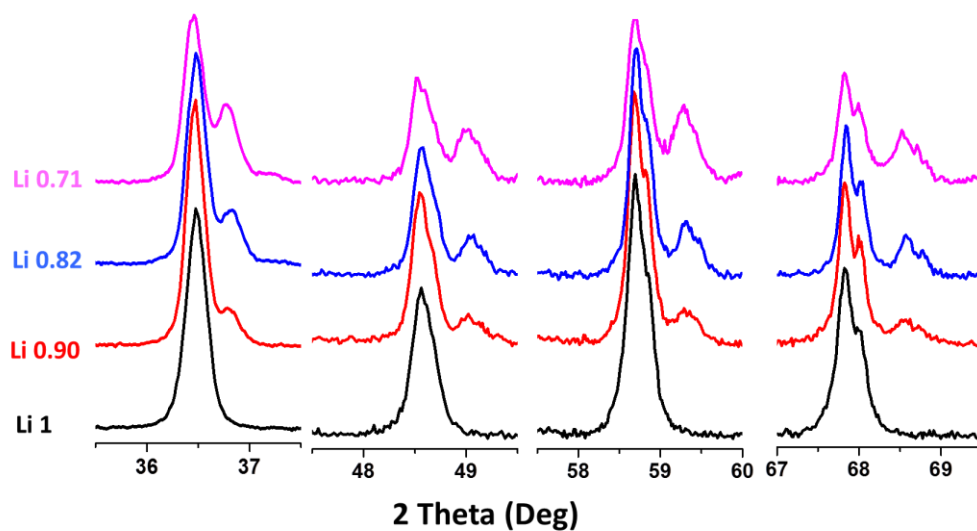
Lawrence Berkeley National Laboratory

Berkeley, California 94720 USA

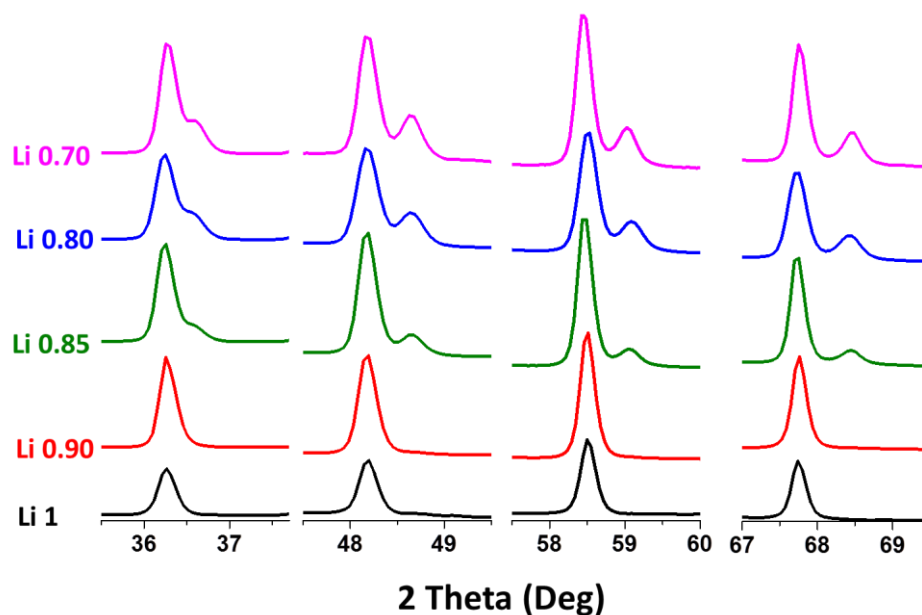
Supporting information

Kuppan et al. Supplementary Figure 1. Room-temperature XRD patterns of $\text{Li}_x\text{Mn}_{1.5}\text{Ni}_{0.5}\text{O}_4$ prepared from: a) chemical and b) electrochemical delithiation.

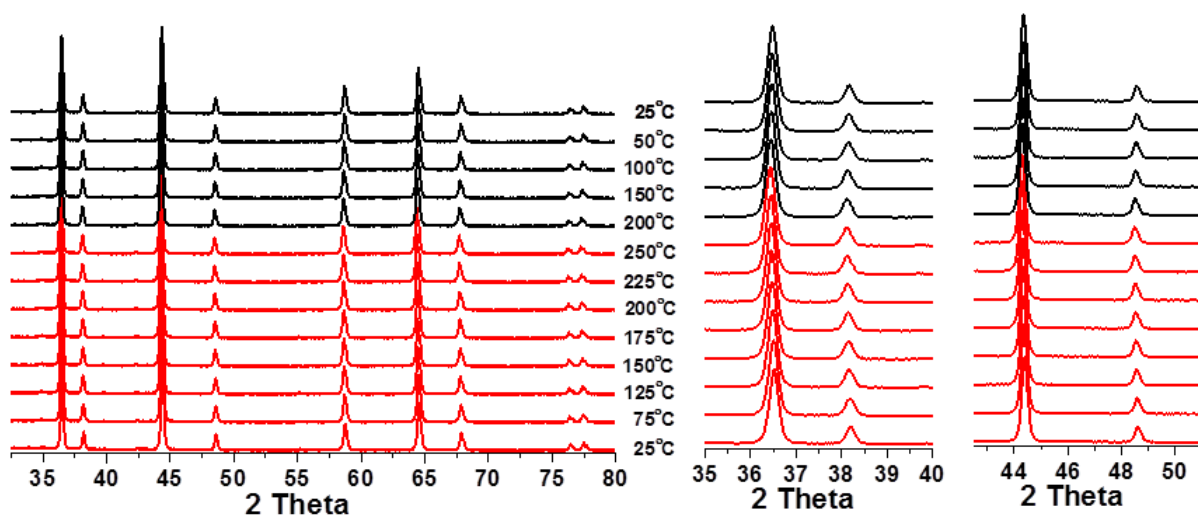
a)



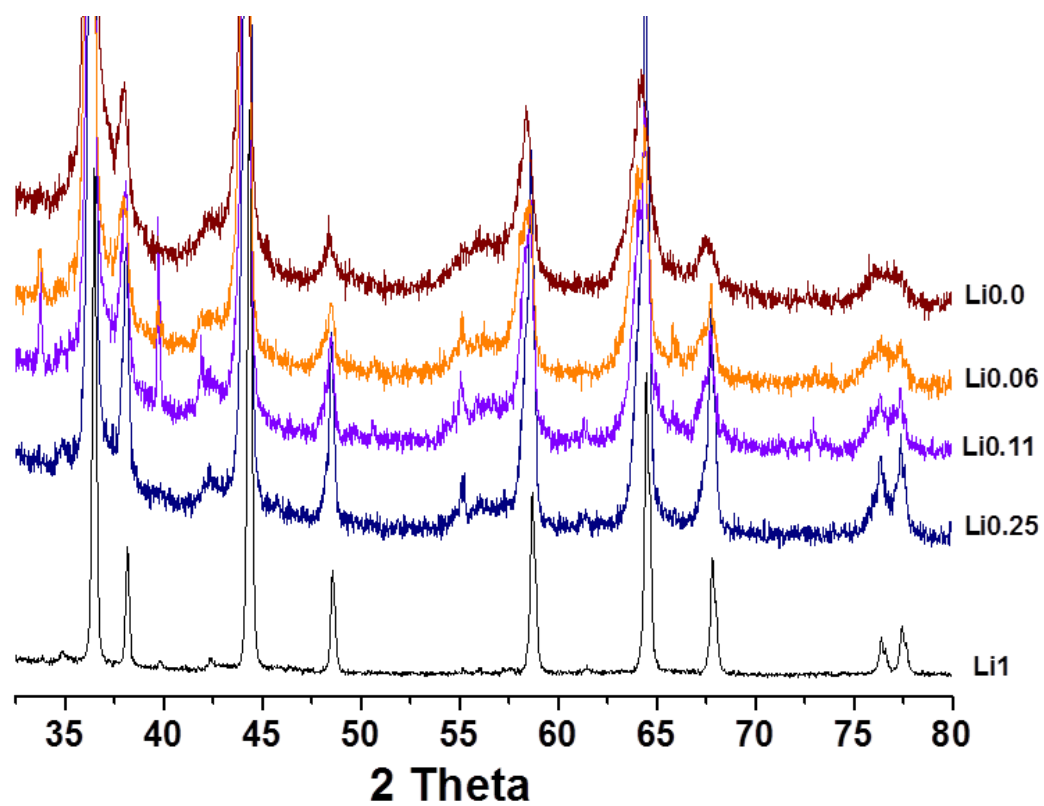
b)



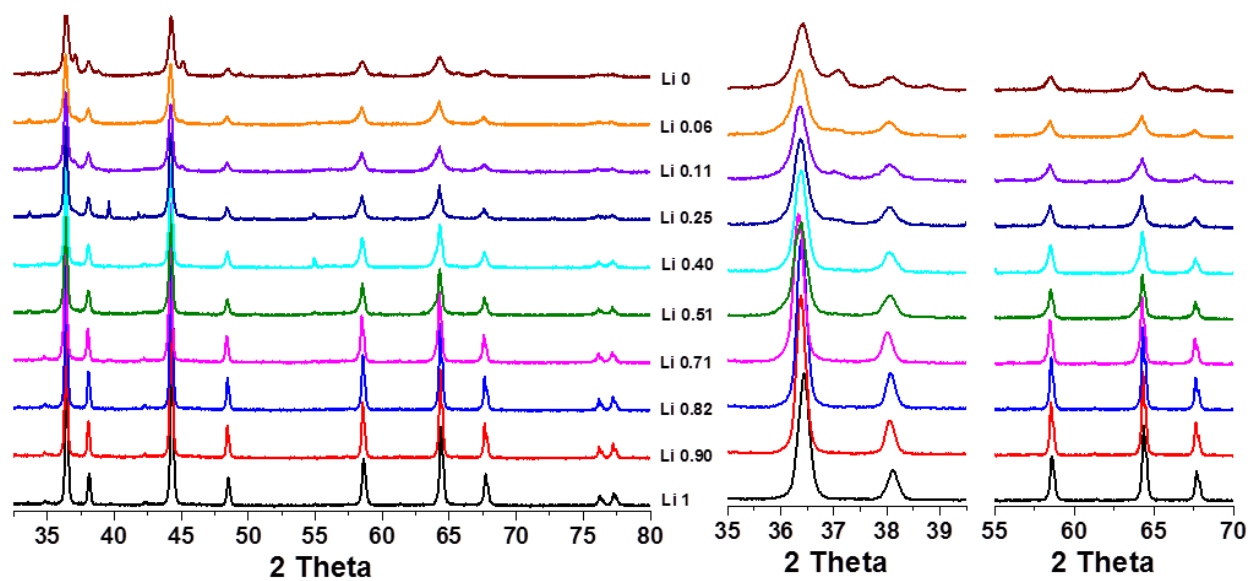
Kuppan et al. Supplementary Figure 2. Temperature-controlled XRD patterns of the pristine LMNO sample



Kuppan et al. Supplementary Figure 3. Room-temperature XRD patterns of the cooled samples with the indicated Li content.



Kuppan et al. Supplementary Figure 4. XRD patterns of the $\text{Li}_x\text{Mn}_{1.5}\text{Ni}_{0.5}\text{O}_4$ crystal samples collected at 265°C.



Kuppan et al. Supplementary Table 1. Rwp, Rexp and goodness of fit χ^2 (GOOF) of the TXRD pattern refinements.

		x=1			x=0.9			x=0.82			
Heating Temp (°C)	Rwp(%)	Rexp(%)	GOOF		Rwp(%)	Rexp(%)	GOOF		Rwp(%)	Rexp(%)	GOOF
25	6.96	4.92	1.41		6.07	4.81	1.26		6.25	4.81	1.3
75	7.05	4.93	1.43		6.24	4.84	1.29		6.43	4.82	1.33
125	7.22	4.94	1.46		6.06	4.85	1.25		6.89	4.83	1.42
150	7.18	4.93	1.45		6.13	4.86	1.26		6.73	4.84	1.39
175	7.12	4.93	1.44		6.21	4.87	1.28		6.79	4.84	1.4
200	6.98	4.94	1.41		6.53	4.87	1.34		6.87	4.84	1.42
225	7.06	4.94	1.43		6.57	4.88	1.35		7.32	4.84	1.5
250	7.04	4.94	1.42		6.68	4.88	1.37		7.36	4.85	1.52
Cooling Temp (°C)											
200	7.15	4.95	1.45		6.82	4.87	1.4		7.26	4.83	1.5
150	7.09	4.94	1.44		6.89	4.87	1.4		7.29	4.83	1.5
100	7.06	4.92	1.43		6.87	4.85	1.4		7.24	4.83	1.5
50	7.18	4.91	1.46		6.75	4.85	1.39		7.25	4.81	1.5
25	6.97	4.9	1.42		6.76	4.84	1.4		6.88	4.81	1.43
		x=0.71				x=0.51				x=0.40	
Heating Temp (°C)	Rwp(%)	Rexp(%)	GOOF		Rwp(%)	Rexp(%)	GOOF		Rwp(%)	Rexp(%)	GOOF
25	5.8	4.79	1.21		5.47	4.78	1.14		6.29	4.98	1.26
75	5.77	4.8	1.2		5.58	4.8	1.16		6.11	4.99	1.22
125	5.81	4.81	1.23		5.59	4.8	1.16		6.33	4.99	1.27
150	5.8	4.81	1.28		5.78	4.81	1.2		6.11	4.99	1.22
175	7.59	4.8	1.58		5.41	4.81	1.2		5.88	5	1.18
200	8.74	4.8	1.82		7.52	4.81	1.56		6.74	4.99	1.35
225	6.63	4.79	1.38		8.73	4.8	1.82		7.87	4.99	1.58
250	6.48	4.79	1.35		6.72	4.8	1.4		7.55	4.99	1.51
Cooling Temp (°C)											
200	6.63	4.78	1.39		6.74	4.79	1.4		6.71	4.78	1.41
150	6.81	4.78	1.4		6.82	4.78	1.43		6.13	4.86	1.26
100	6.71	4.78	1.41		6.66	4.78	1.39		6.53	4.87	1.34
50	6.54	4.76	1.37		6.46	4.78	1.36		6.11	4.99	1.22
25	6.5	4.76	1.37		6.7	4.75	1.41		6.88	4.81	1.43
		x=0.25				x=0.11				x=0.06	
Heating Temp (°C)	Rwp(%)	Rexp(%)	GOOF		Rwp(%)	Rexp(%)	GOOF		Rwp(%)	Rexp(%)	GOOF
25	5.7	5.13	1.1		6.99	5.01	1.39		6.99	5.01	1.39
75	5.84	5.16	1.13		7.15	5.03	1.42		7.15	5.03	1.42
125	5.95	5.17	1.15		7.27	5.04	1.43		7.27	5.04	
150	5.36	5.17	1.04		7.32	5.04	1.45		7.32	5.04	1.45
175	5.6	5.16	1.1		7.46	5.04	1.48		7.46	5.04	1.48
200	6.42	5.16	1.25		5.79	5.03	1.15		5.79	5.03	1.15
225	6.73	5.15	1.31		7.3	5.03	1.47		7.3	5.03	1.47
250	6.96	5.14	1.55		6.35	5	1.27		6.35	5	1.27
Cooling Temp (°C)											
200	6.84	5.13	1.33		6.94	4.99	1.39		6.94	4.99	1.39
150	6.91	5.12	1.35		6.98	4.98	1.4		6.98	4.98	1.4
100	6.91	5.1	1.35		7.01	4.97	1.41		7.01	4.97	1.41
50	6.85	5.08	1.35		7.13	4.96	1.44		7.13	4.96	1.44
25	6.85	5.07	1.35		6.98	4.98	1.4		7.13	4.96	1.44
		x=0									
Heating Temp (°C)	Rwp(%)	Rexp(%)	GOOF								
25	6.93	5.23	1.33								
75	7.15	5.24	1.36								
125	7.21	5.25	1.37								
150	7.63	5.26	1.45								
175	8.25	5.25	1.57								
200	7.16	5.23	1.37								
225	6.84	5.22	1.35								
250	6.86	5.19	1.32								
Cooling Temp (°C)											
200	6.62	5.19	1.28								
150	6.69	5.18	1.28								
100	6.5	5.17	1.26								
50	6.5	5.14	1.27								
25	6.5	5.13	1.27								