

Ultra-rapid microwave synthesis of $\text{Li}_{3-x-y}\text{M}_x\text{N}$ (M= Co, Ni and Cu) nitridometallates.

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SUPPLEMENTARY INFORMATION

Table S1 Lattice parameters and cell volumes obtained from indexed powder X-ray data for samples (1-7).

<i>Sample</i>	M	<i>x</i>	<i>a/Å</i>	<i>c/Å</i>	<i>V/Å³</i>
1	Ni	0.1	3.668(2)	3.8416(5)	44.77(2)
2	Ni	0.22	3.688(1)	3.741(4)	44.05(5)
3	Ni	0.29	3.697(6)	3.72(2)	44.08(2)
4	Co	0.09	3.667(3)	3.8267(8)	44.56(4)
5	Co	0.21	3.678(2)	3.804(3)	44.57(4)
6	Co	0.3	3.697(7)	3.772(2)	44.65(9)
7	Cu	0.11	3.670(3)	3.806(7)	44.32 (4)

Table S2 Thermal displacement parameters for atoms in samples 1-7.

Atoms	$U^a \times 100$ $/\text{\AA}^2$	1	2	3	4	5	6	7
M/Li(1)	U_i/U_e	2.64	1	0.14	1.58	3.90	2.49	1.33
(0,0,0.5)	U_{11}	3.8(9)	-	0.2(1)	2.1(3)	4.6(7)	3.9(4)	2.5(3)
	U_{33}	0.2(9)	-	0.1(3)	0.4(4)	2.31(3)	1.4(1)	1.5(3)
N	U_i/U_e	1.55	2.35	2.98	1.21	1.58	2.33	1.69
(0,0,0)	U_{11}	1.33(6)	1.56(5)	1.96(5)	1.00(5)	1.38(7)	1.99(4)	1.08(4)
	U_{33}	1.9(1)	3.9(1)	4.97(2)	1.60(7)	2.0(1)	2.98(7)	2.9(8)
Li(2)	U_i/U_e	3.59	4.28	3.82	2.37	2.31	3.12	4.79
(0.3333, 0.6667, 0)	U_{11}	1.6(3)	2.7(3)	2.0(2)	1.5(2)	1.5(3)	2.3(2)	1.6(2)
	U_{33}	7.5(9)	7.3(9)	7.4(8)	4.0(4)	3.9(7)	4.7(4)	9.8(8)

^a $U_{11} = U_{22} = 2 U_{12}$ and $U_{13} = U_{23} = 0$.



Fig. S1 Photograph showing a reaction in progress demonstrating the occurrence of an orange-yellow glow following Li evaporation.

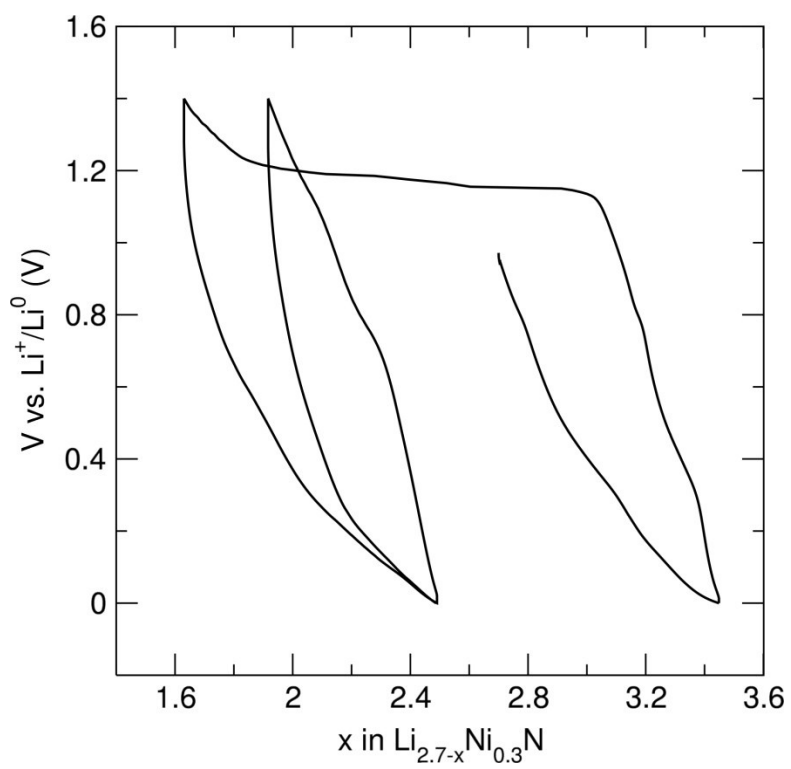


Fig. S2 First two charge/discharge cycles of $\text{Li}_{2.7-x}\text{Ni}_{0.3}\text{N}$ (3) between 0 and 1.4 V at a C/30 rate.

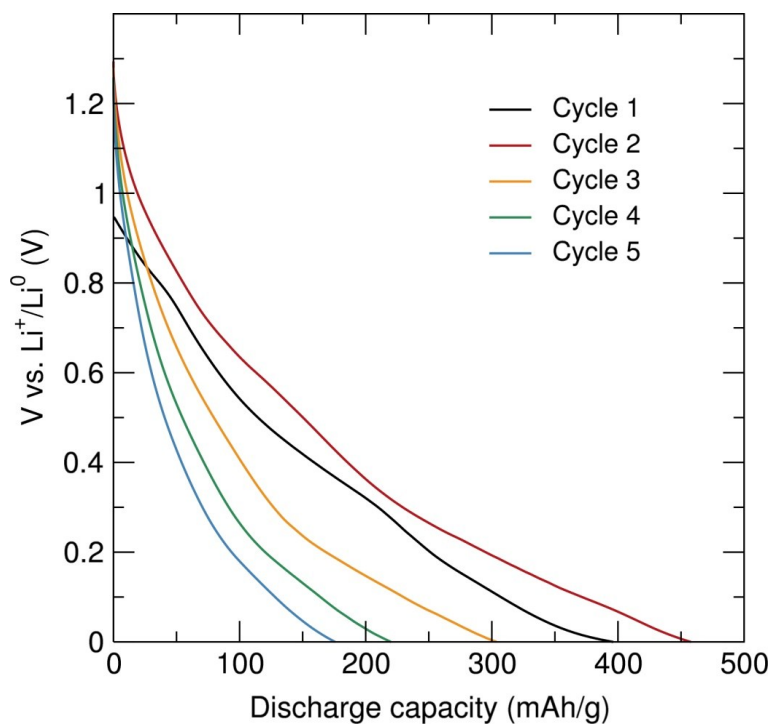


Fig. S3 Discharge capacity for the first five cycles of $\text{Li}_{2.7-x}\text{Ni}_{0.3}\text{N}$ (3) tested galvanostatically against lithium metal between 0 and 1.4 V at a C/30 rate.

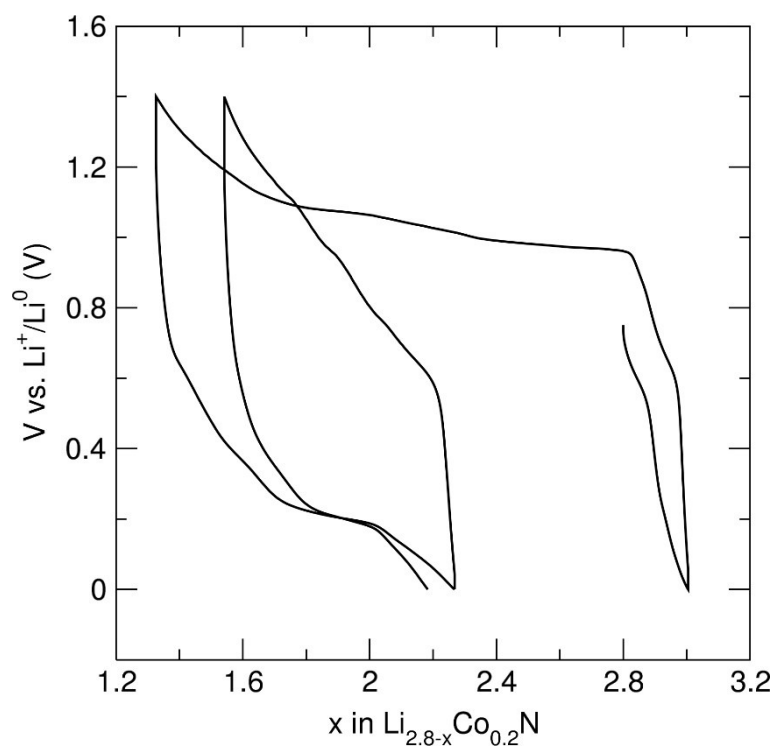


Fig. S4 First two charge/discharge cycles of $\text{Li}_{2.8-x}\text{Co}_{0.2}\text{N}$ (5) between 0 and 1.4 V at a C/30 rate.

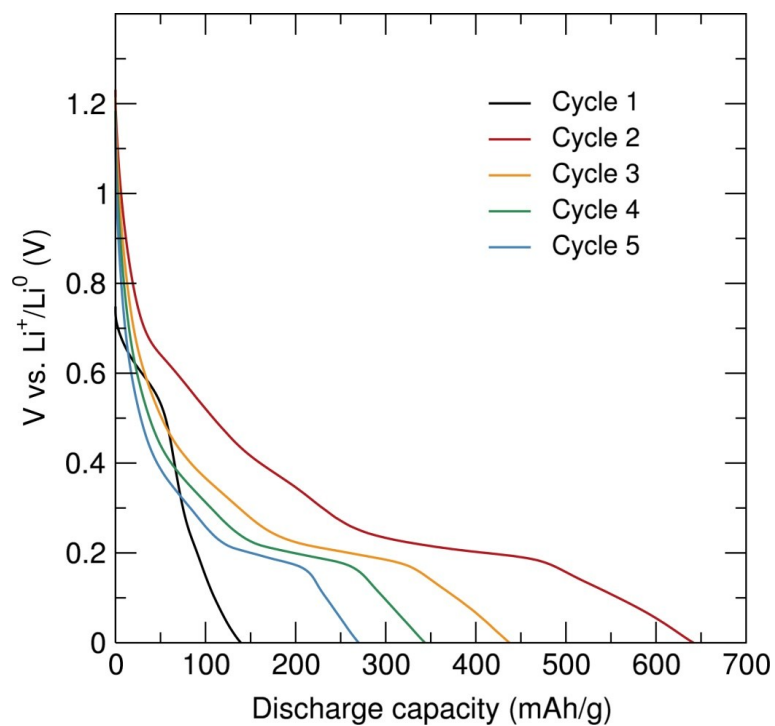


Fig. S5 Discharge capacity for the first five cycles of $\text{Li}_{2.8-x}\text{Co}_{0.2}\text{N}$ (5) tested galvanostatically against lithium metal between 0 and 1.4 V at a C/30 rate.