

Modulating the Li⁺/Ni²⁺ replacement and electrochemical performance optimizing of layered lithium-rich Li_{1.2}Ni_{0.2}Mn_{0.6}O₂ by minor Co dopant

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Table S1 The transition metal composition ratio of the experimental and theoretic value for specimens z0, z2, z4, z10

	experimental(Mn: Ni: Co)	theoretic (Mn: Ni: Co)
z0	0.600 : 0.205	0.600 : 0.200
z2	0.590 : 0.186 : 0.021	0.590 : 0.190 : 0.021
z4	0.580 : 0.183 : 0.041	0.580 : 0.180 : 0.041
z10	0.550 : 0.137 : 0.110	0.550 : 0.137 : 0.110

Table S2 Magnetic parameters for the specimen z0, z2, z4, z10.

	Cp, ^a emu K/mol	θ _p , ^a K	μ _{exp} , ^a μ _B	μ _{theor} , ^b μ _B	M _s , emu/mol	Ni ²⁺ (3b)
z0	1.280	-27.4	3.19	3.25	470.2	3.83%
z2	1.265	-26.6	3.15	3.22	292.3	2.38%
z4	1.250	-26.1	3.13	3.18	250.79	2.04%
z10	1.142	-22.4	2.99	3.07	141.42	1.15%

^a The Cp, θ_p, μ_{exp} are calculated from Curie-Weiss law: H/M=(T-θ_p)/Cp, and the relation Cp=N μ_{exp}²/(3k_B)

^b The theoretical magnetic moments μ_{theor} is got by assuming Mn⁴⁺(S=3/2), Ni²⁺(S=1) and Co³⁺(S=0, LS)

Table S3 Fitting parameters for the EIS spectrum

	R _e (Ω)	R _s (Ω)	R _{ct} (Ω)	D _{Li+} (cm ² s ⁻¹)
z0	6.293	821	1981	2.11E-16
z2	14.7	422.8	722.9	1.29E-15
z4	3.902	119.4	134.7	5.41E-15
z10	8.967	206.5	293.7	4.01E-15

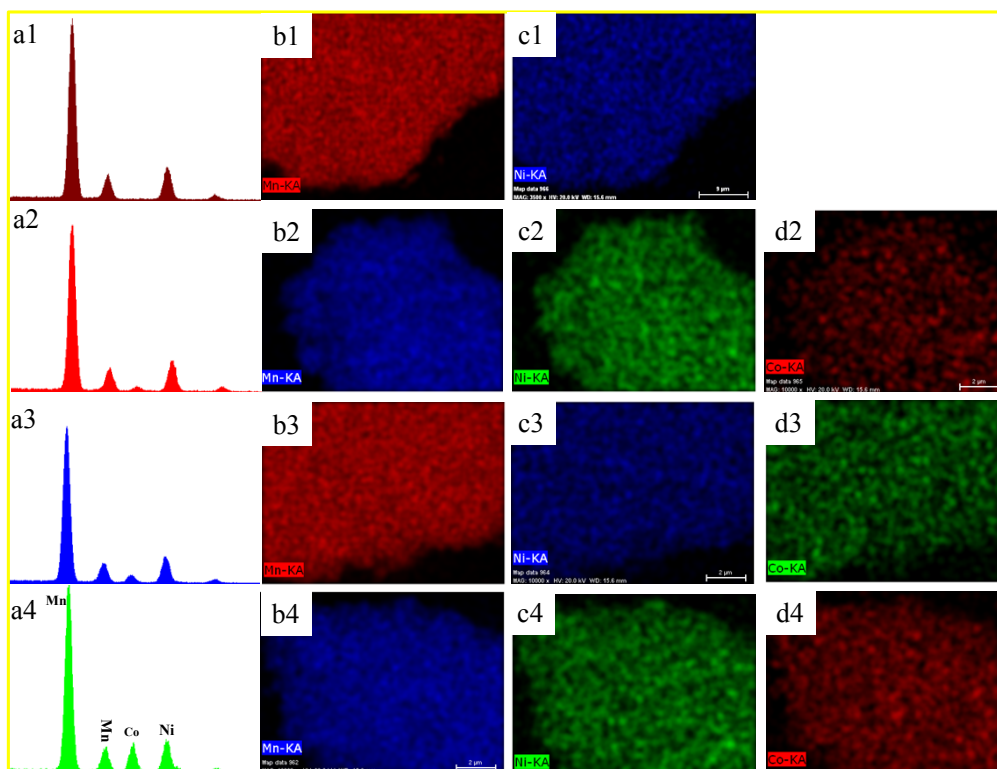


Fig. S1 Energy dispersive X-ray (EDX) spectroscopy of all the specimens z0(1), z2(2), z4(3), z10(4): (a) Intensity plots and (b ~d) EDX mapping for Mn (b1~b4), Ni(c1~c4), Co(d2~d4)

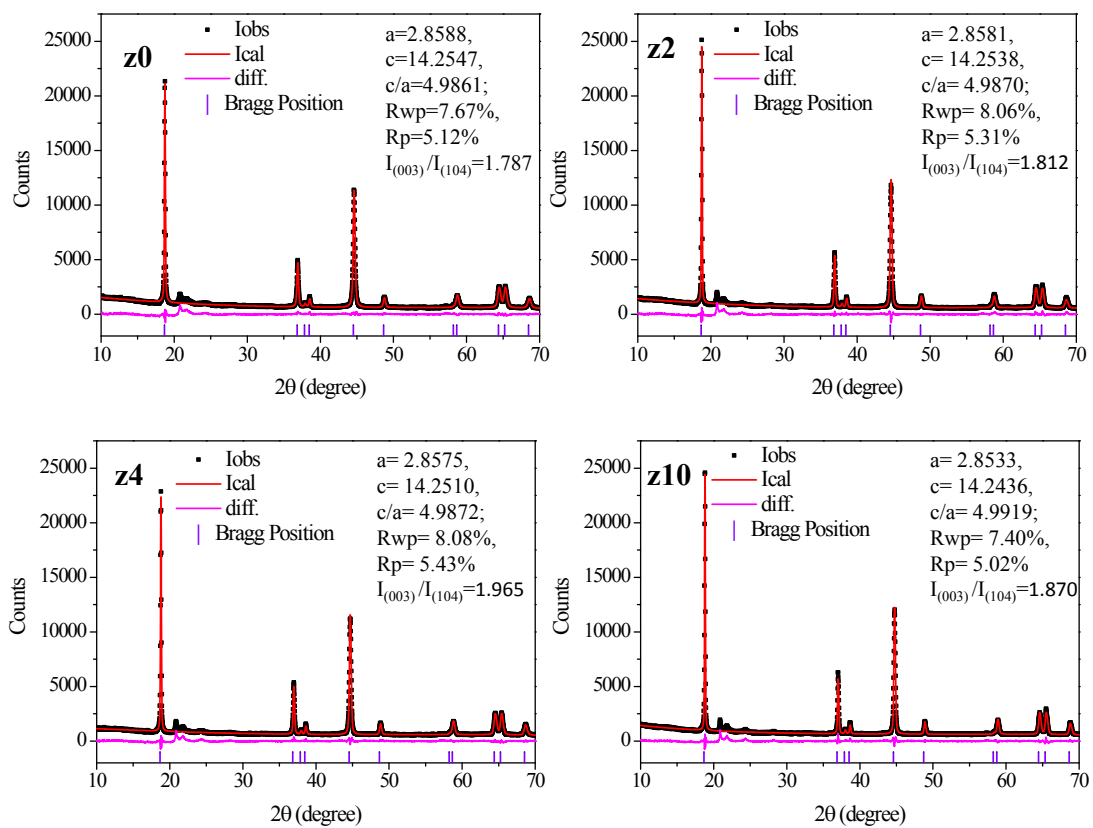


Fig. S2 XRD refinement results for the specimens for z0, z2, z4, z10 by using the TOPAS software.

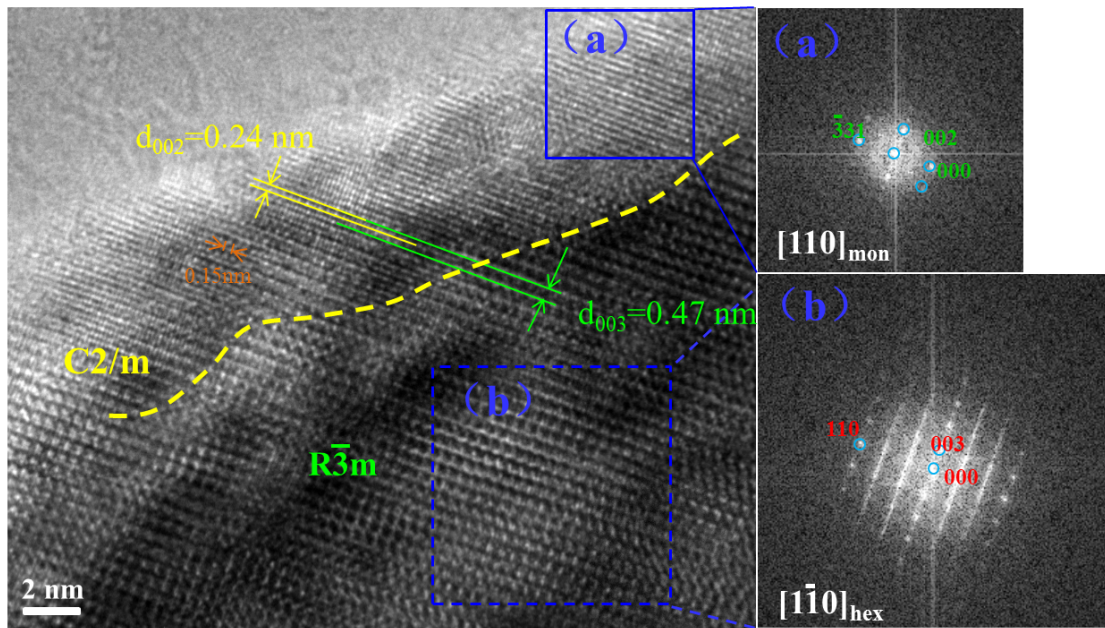


Fig.S3 HRTEM images for specimen z0 and FFT(Fast Fourier Transformed) images for the regions indicted by blue box(a) at the margin and blue dotted box(b) inside the particle. The miller indexes are denoted according to the C2/m space group(green) and the R $\bar{3}$ m space group (red).

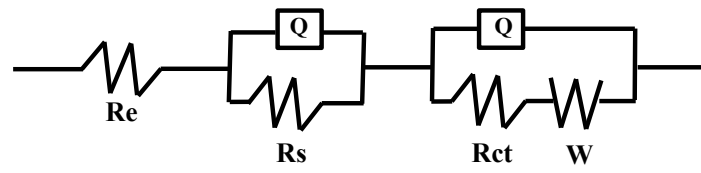
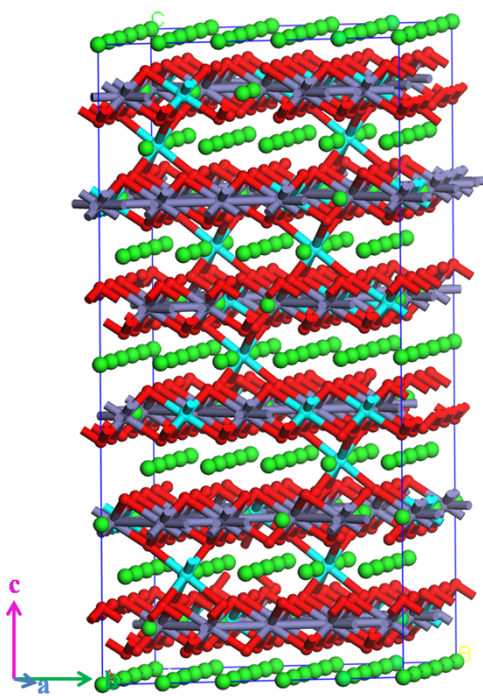
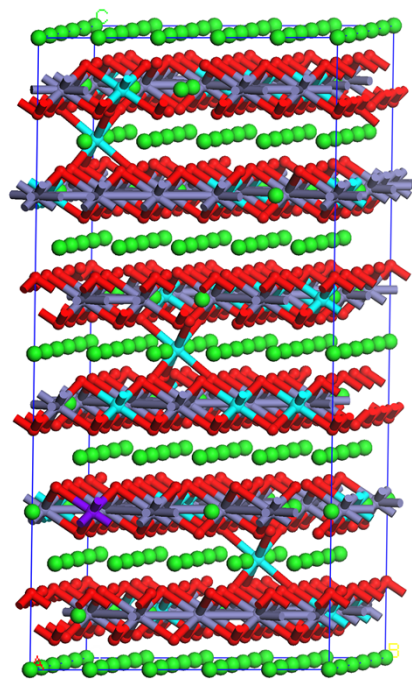


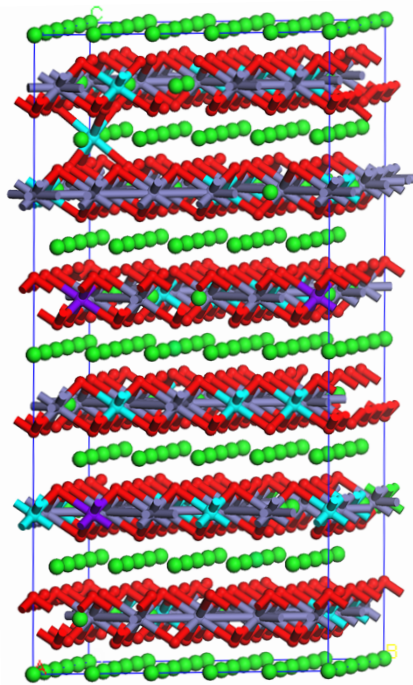
Fig.S4 Equivalent circuit used in the EIS fitting



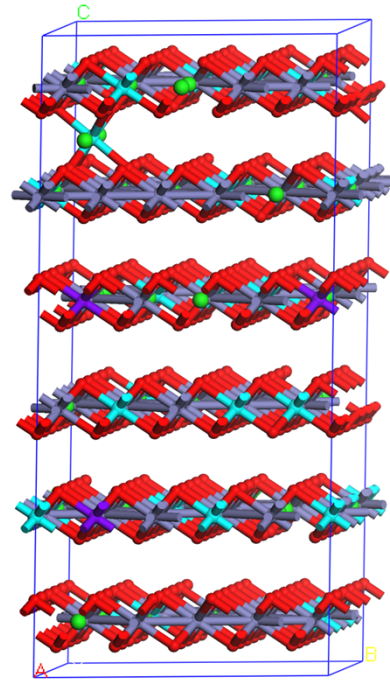
z0



z4



z10



z10
delithiated

Fig.S5 Ball-and-stick models for the specimen z0, z4, z10 and the delithiated state of z10.