Supporting Information

Fe Doping in $LiMn_{1.5}Ni_{0.5}O_4$ by Atomic Layer Deposition Followed by Annealing: Depths and Occupation Sites

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This supporting information file includes (1) X-ray diffraction (XRD) patterns of uncoated $LiMn_{1.5}Ni_{0.5}O_4$ (LMNO), and LMNO after FeO_x atomic layer deposition (ALD) and post-annealed particles at 500 °C (Fe500), 600 °C (Fe600), 700 °C (Fe700), and 800 °C (Fe800), respectively; (2) cross-sectional scanning electron microscopy (SEM) image of one Fe700 particle; (3) X-ray photoelectron spectroscopy (XPS) survey scans of $Li_4Ti_5O_{12}$ (LTO) and LMNO of UC, Fe650, and Fe700 after 200 cycles of charge/discharge in LMNO-LTO full cells; (4) XPS spectra of C 1s core levels of LMNO and LTO of UC, Fe650, and Fe700 in LMNO-LTO full cells after 200 cycles of charge/discharge; and (5) the fitted ^{57}Fe Mössbauer spectroscopic values for Isomer Shift (IS), Quadrupole Splitting (QS), and Hyperfine magnetic splitting (H) of Fe650 and Fe700 samples.

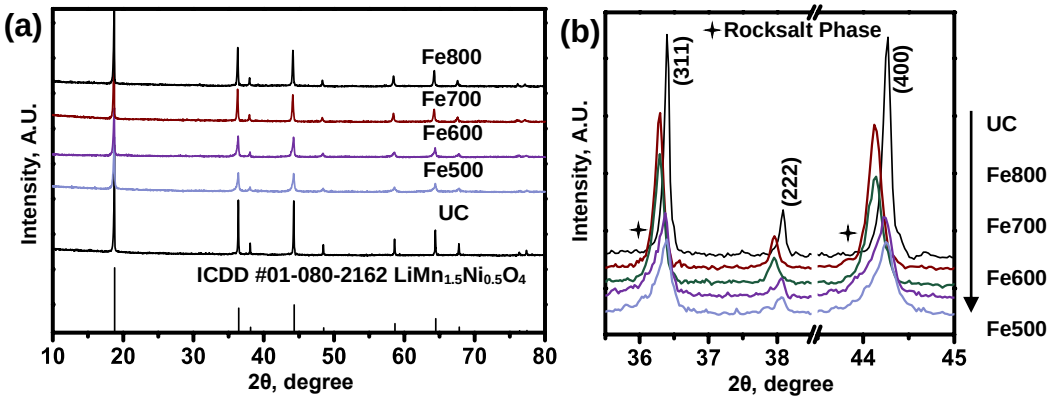

Figure S1. (a) XRD patterns of uncoated LMNO (UC), Fe500, Fe600, Fe700, and Fe800 particles and (b) the magnified patterns between 35.5 degree and 45 degree of 2θ.

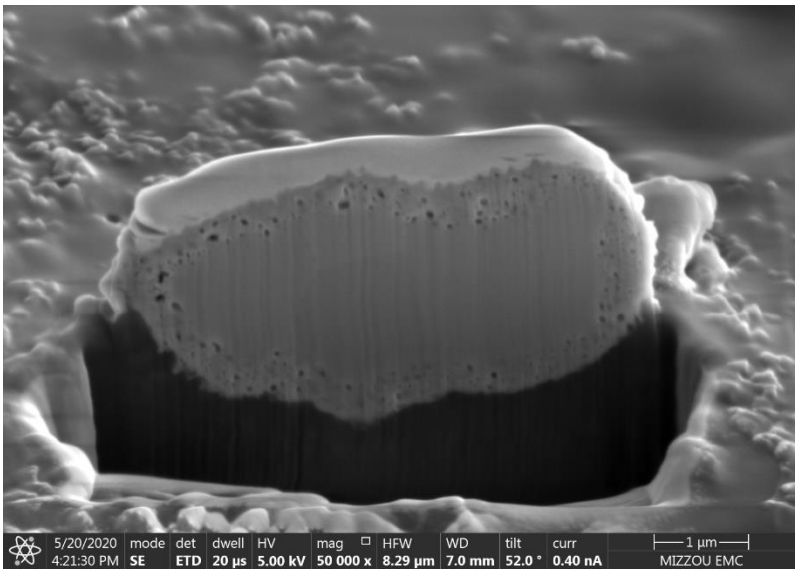

Figure S2. Cross-sectional SEM image of one Fe700 particle.

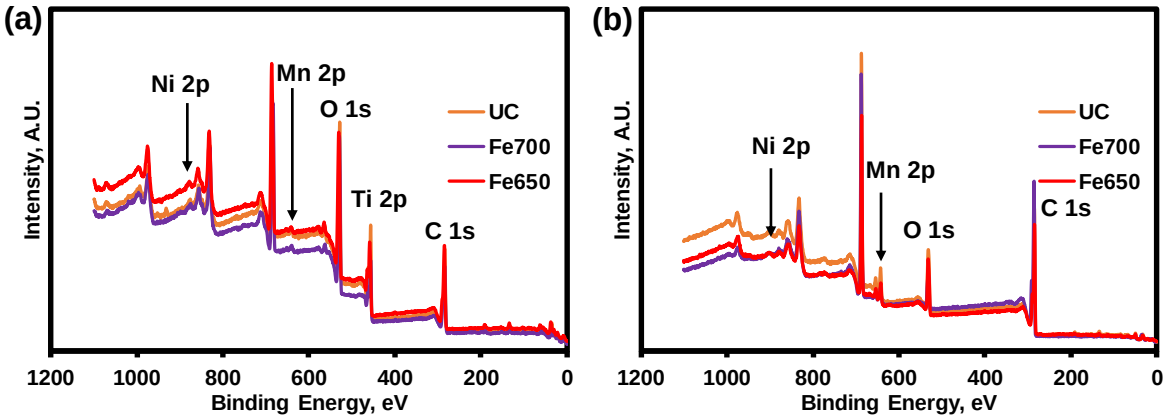

Figure S3. XPS survey scans of (a) LTO and (b) LMNO of UC, Fe650, and Fe700 after 200 cycles of charge/discharge in LMNO-LTO full cells.

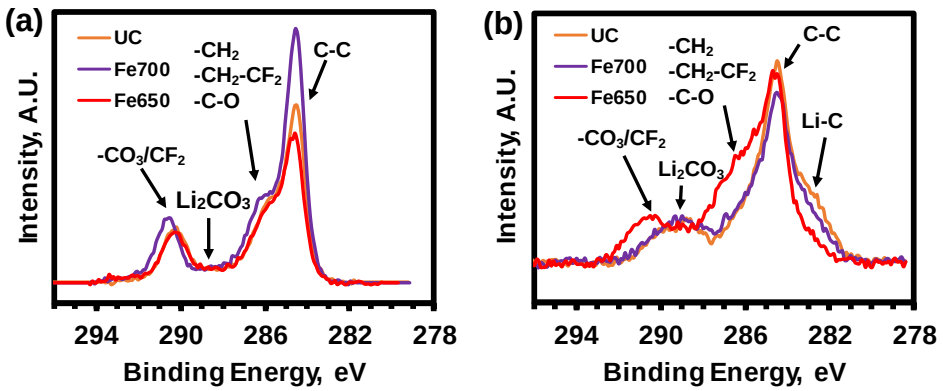

Figure S4. XPS spectra of C 1s core levels of (a) LMNO and (b) LTO of UC, Fe650, and Fe700 after 200 cycles of charge/discharge in LMNO-LTO full cells.

Table S1. The fitted ^{57}Fe Mössbauer spectroscopic values for Isomer Shift (IS), Quadrupole Splitting (QS), and Hyperfine magnetic splitting (H) of Fe650 and Fe700 samples.

Fe 650

Sites	IS (δ) ($mm.s^{-1}$)	QS (ΔE_Q) ($mm.s^{-1}$)	Width ($mm.s^{-1}$)	Hyperfine magnetic field, H (k Oe)	Site population (%)
Doublet site-1	0.333(2)	0.779(3)	0.29(3)		37.1
Doublet site-2	0.216(5)	0.440(1)	0.38(9)		18.1
Sextet site	0.274(3)		0.35(8) (W3)	454.3(3)	44.8

Fe 700

Sites	IS(δ) ($mm.s^{-1}$)	QS (ΔE_Q) ($mm.s^{-1}$)	Width ($mm.s^{-1}$)	Site population (%)
Doublet site-1	0.322(8)	0.792(2)	0.28(1)	65.2
Doublet site-2	0.244(2)	0.375(3)	0.27(3)	34.8