

Supporting Information

Positive Role of Fluorine Impurity in Recovered $\text{LiNi}_{0.6}\text{Co}_{0.2}\text{Mn}_{0.2}\text{O}_2$ Cathode Materials

Yadong Zheng ^a, Ruihan Zhang ^a, Panawan Vanaphuti ^a, Yangtao Liu ^a,
Zhenzhen Yang ^b, and Yan Wang ^{a,*}

^a Department of Mechanical Engineering, Worcester Polytechnic Institute, Worcester, MA 01609, USA

^b Chemical Sciences and Engineering Division, Argonne National Laboratory, Lemont, IL 60439, USA

*Correspondence: yanwang@wpi.edu (Yan Wang)

6 Pages, 6 Figures and 5 Tables

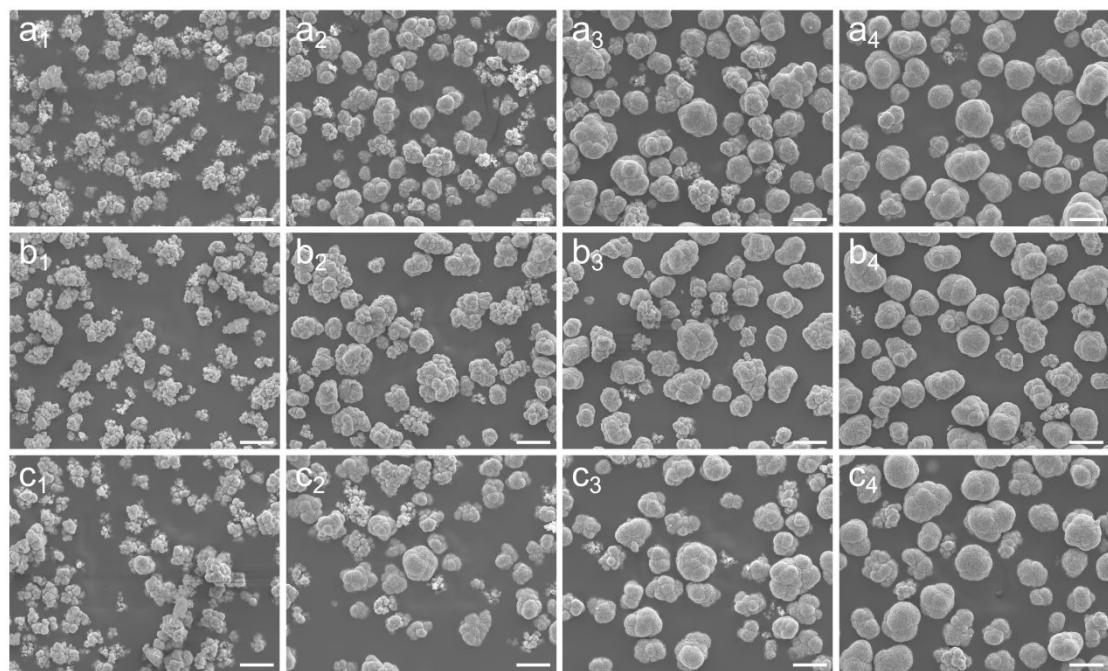


Figure S1. SEM images of precursors for 0.2FNCM (a₁-a₄), 1FNCM (b₁-b₄) and 5FNCM (c₁-c₄) at 3hr, 6hr, 9hr and 12hr (scale bar 10μm).

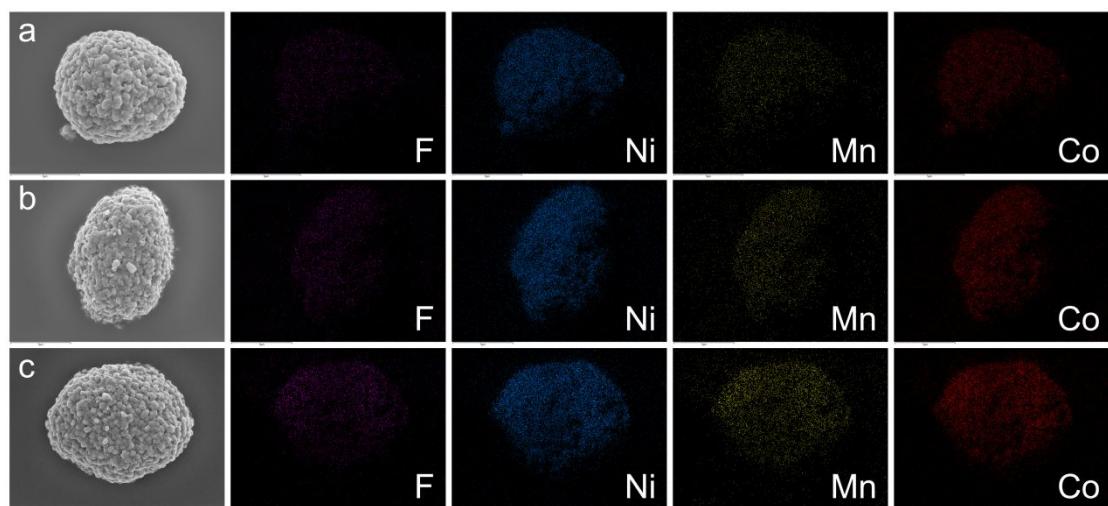


Figure S2. SEM-EDS multi-element mapping of cathodes for (a) 0.2FNCM, (b) 1FNCM and (c) 5FNCM.

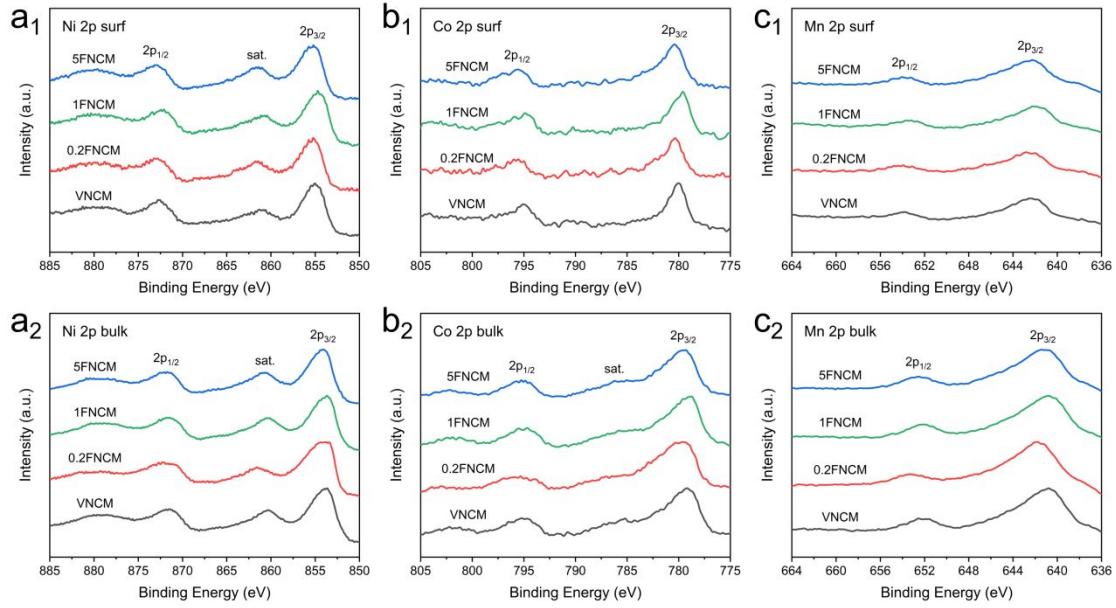


Figure S3. High-resolution XPS spectra of (a₁, a₂) Ni 2p, (b₁, b₂) Co 2p and (c₁, c₂) Mn 2p in cathodes; Upper row (a₁, b₁, c₁) for surface and lower row (a₂, b₂, c₂) for bulk results.

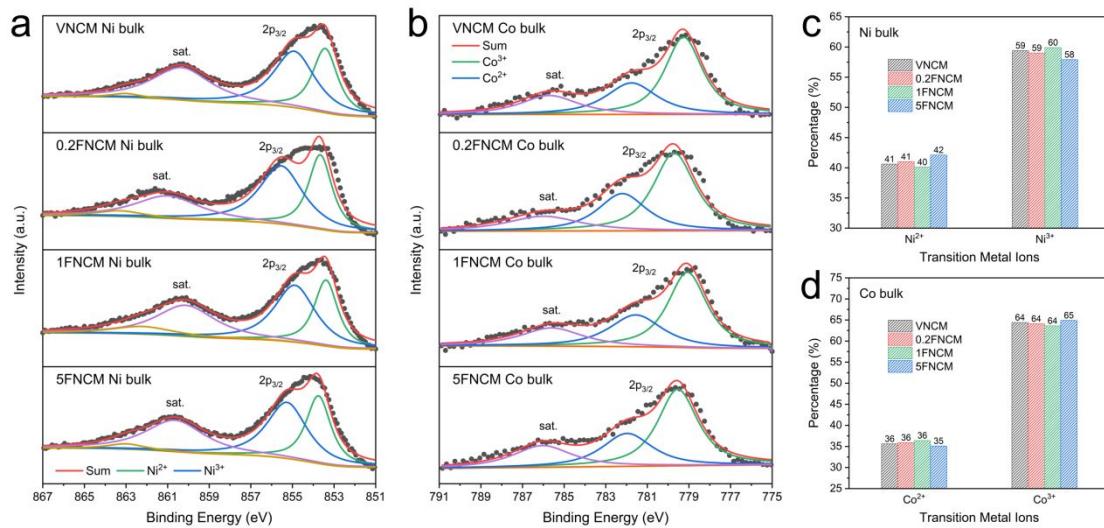


Figure S4. XPS deconvolution profiles of (a) Ni 2p, (b) Co 2p in bulk of cathodes; Percentage of (c) Ni²⁺, Ni³⁺ ions and (d) Co²⁺, Co³⁺ ions in bulk of cathodes.

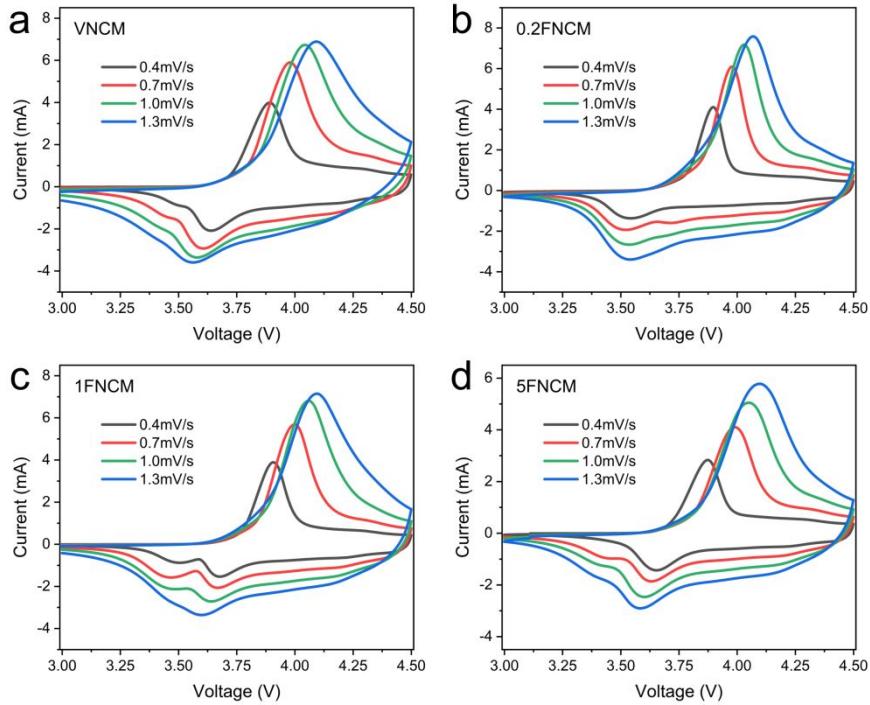


Figure S5. CV profiles of (a) VNCM, (b) 0.2FNCM, (c) 1FNCM and (d) 5FNCM under different scan rates.

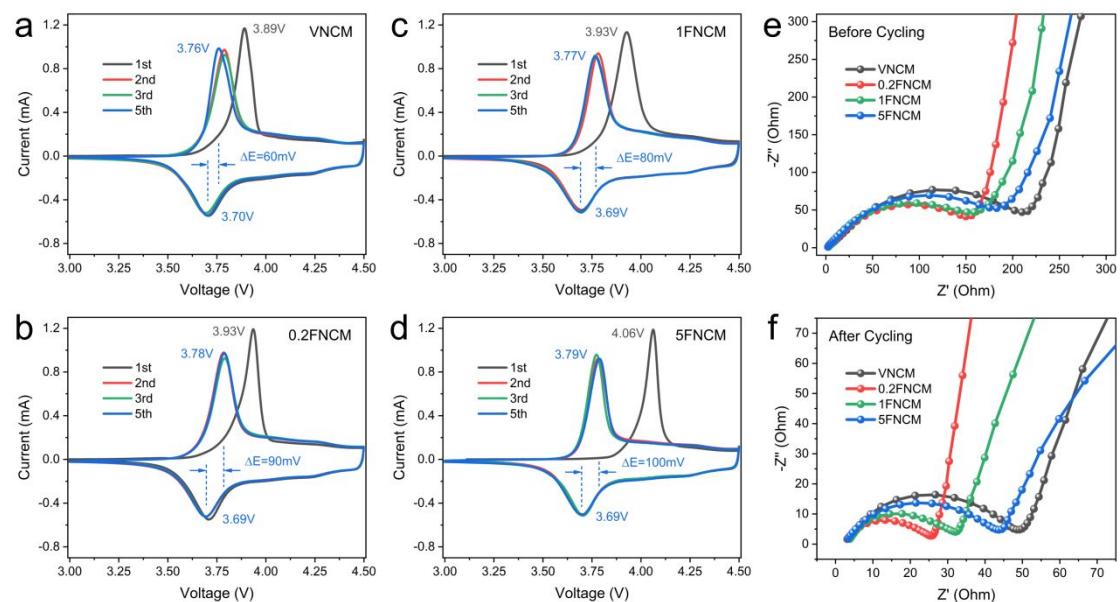


Figure S6. CV curves of first five cycles for (a) VNCM, (b) 0.2FNCM, (c) 1FNCM and (d) 5FNCM cathode samples; EIS plots of different electrodes (e) before and (f) after cycling (150 cycles).

Table S1. Tap density (g/ml) of the precursors at different reaction times.

Sample	3hrs	6hrs	9hrs	12hrs
VNCM	0.68	1.15	1.52	1.85
0.2FNCM	0.94	1.47	1.73	1.93
1FNCM	0.92	1.47	1.72	1.93
5FNCM	0.78	1.41	1.65	1.88

Table S2. ICP-MS results of the synthesized cathode materials in molar ratio.

Sample	Li (%)	Ni (%)	Mn (%)	Co (%)	Na (%)
VNCM	103.6	59.7	19.9	20.4	0
0.2FNCM	102.8	59.3	19.9	20.9	0
1FNCM	102.6	59.4	19.8	20.8	0
5FNCM	103.6	58.8	20.1	21.1	0

Table S3. Diffusion results obtained from Randles-Sevcik equation.

Sample	Slope I_p^2/v ($10^{-3}A^2s/V$)		Diffusivity D_{Li} ($10^{-11}cm^2/s$)	
	Anodic	Cathodic	Anodic	Cathodic
VNCM	34.998	9.461	15.7	4.24
0.2FNCM	45.497	10.791	20.4	4.83
1FNCM	40.635	9.957	18.2	4.46
5FNCM	28.288	7.249	12.7	3.25

Table S4. Parameters data based on EIS fitting curves.

Sample	Status	R _s (Ω)	R _{ct} (Ω)
VNCM	before/after cycling	2.3/3.3	209/48
0.2FNCM		2.1/2.3	158/24
1FNCM		2.2/3.1	162/29
5FNCM		1.6/2.5	188/42

Table S5. Rate performance of all samples at different current densities.

C-Rate	Average Discharge Capacity (mAh/g)			
	VNCM	0.2FNCM	1FNCM	5FNCM
0.05C	175.3	178.7	177.2	175.5
0.1C	174.3	178.9	176.6	174.3
0.2C	169.4	173.9	173.8	170.2
0.5C	161.4	165.7	165.6	161.8
1C	152.9	157.9	157.9	154.6
2C	142.4	148.0	146.8	143.2
3C	132.1	139.3	138.2	134.1
5C	117.4	125.3	122.2	118.9