Supporting Information

Cobalt-Free High-Energy Ternary Cathode $LiNi_{0.9}Fe_{0.05}Mn_{0.05}O_2$: Synthesis and Electrochemical Performance for High-Energy Lithium-Ion Batteries

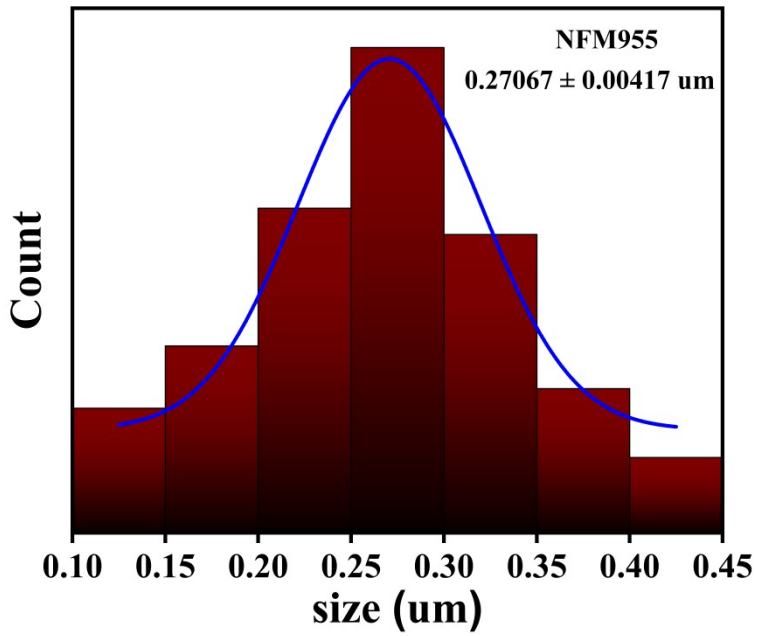

Figure S1 Particle size distribution diagram of NFM955 cathode material synthesized under calcination condition of 750°C for 20 h

Table S1. Rietveld refinement data of NFM955 samples.

sample	NFM 725℃ 20 h	NFM 775℃ 20 h	NFM 750℃ 20 h	NFM 750℃ 16 h	NFM 750℃ 24 h
a(Å)	2.87987	2.87800	2.88657	2.87248	2.88105
c(Å)	14.22269	14.21997	14.26459	14.18892	14.22865
V(Å^3)	102.155	102.002	102.933	101.390	102.281
c/a	4.93865	4.94092	4.94171	4.93960	4.93870
Ni in Li site	5.66%	8.80%	4.52%	7.89%	8.12%

Table S2. First charge-discharge data of NFM955 samples at 0.1C

sample	Initial Charge Specific Capacity (mAh/g)	Initial Discharge Specific Capacity (mAh/g)	Coulombic Efficiency (%)
NFM 725℃ 20 h	225.86	194.35	86.05
NFM 775℃ 20 h	218.59	189.28	86.59
NFM 750℃ 20 h	226.73	197.85	87.26
NFM 750℃ 16 h	229.35	192.59	83.97
NFM 750℃ 24 h	219.82	185.60	84.43

Table S3. The electrochemical performance data of NFM955 cathode materials at 0.2 C

sample	Initial Discharge Specific Capacity (mAh/g)	100th discharge specific capacity (mAh/g)	Capacity Retention Rate (%)
NFM 725℃ 20 h	181.90	150.92	82.97
NFM 775℃ 20 h	179.45	145.49	81.08
NFM 750℃ 20 h	194.89	168.17	86.29
NFM 750℃ 16 h	180.65	152.80	84.58
NFM 750℃ 24 h	179.82	149.00	82.86

Table S4. The electrochemical performance data of NFM955 cathode materials at 0.5 C

sample	Initial Discharge Specific Capacity (mAh/g)	100th discharge specific capacity (mAh/g)	Capacity Retention Rate (%)
NFM 725℃ 20 h	163.69	151.77	92.72
NFM 775℃ 20 h	162.99	143.06	87.77
NFM 750℃ 20 h	167.60	155.45	92.75
NFM 750℃ 16 h	162.44	143.39	88.27
NFM 750℃ 24 h	159.64	145.11	90.89

Table S5. The rate performance data of NFM955 samples

sample	0.1 C	0.2 C	0.5 C	1 C	2 C	5 C	0.1 C	Retention Rate
NFM 725℃ 20 h	194.35	178.37	157.00	134.23	118.68	86.96	175.40	90.24%
NFM 775℃ 20 h	189.28	178.56	163.63	143.77	117.95	80.49	181.53	95.90%
NFM 750℃ 20 h	197.85	189.78	164.42	144.52	131.1	92.87	184.49	93.24%
NFM 750℃ 16 h	192.59	178.7	159.9	137.91	120.54	90.57	175.49	91.12%
NFM 750℃ 24 h	185.60	177.03	161.03	143.94	130.70	99.61	176.87	95.29%

Table S6. EIS fitting parameters of NFM955 cathode materials after the first cycle.

sample	*Rs*(Ω)	*Rf*(Ω)	*Rct*(Ω)	*DLi*+(cm^2s^{-1})
NFM 725℃ 20 h	1.687	19.95	37.37	2.2517×10^{-14}
NFM 775℃ 20 h	1.841	23.19	17.12	6.9921×10^{-14}
NFM 750℃ 20 h	2.139	18.69	16.12	8.1051×10^{-14}
NFM 750℃ 16 h	2.556	25.05	66.96	5.0831×10^{-14}
NFM 750℃ 24 h	3.139	32.89	64.85	1.5136×10^{-14}

TableS7 Compared with the previous circulating properties of related cathode materials.

sample	Synthetic methods	Initial discharge capacity(mAh/g)	Capacity retention(%)	Potential Range (V vS Li^+/Li	Refs
$LiNi_{0.8}Mn_{0.1}Fe_{0.1}O_2$	Co-precipitation+ solid-state	79 @ C/2, 125 @ C/10	51% after 70 cycles @ C/5	3.0 ~ 4.4	[33]
$LiNi_{0.8}Fe_{0.15}Al_{0.05}O_2$	Co-precipitation	180 @ C/3, 190 @ C/10	70% after 100 cycles @C/3	3.0 ~ 4.5	[9]
$LiNi_{0.9}Fe_{0.05}Al_{0.05}O_2$	Modified rheological phase reaction	195 @ C/10	85% after 100 cycles @1 C	3.0 ~ 4.5	[34]
$LiNi_{0.8}Fe_{0.1}Al_{0.1}O_2$	Solid-state	160 @ C/5,180 @ C/10	99.6% after 100 cycles @C/2	3.0 ~ 4.5	[34]
$LiNi_{0.95}Mg_{0.02}Al_{0.03}O_2$	Co-precipitation	176.6 @ C/10, 140.7 @ 1 C, 108.1 @ C/2, 88.4 @ 2 C, 59.1 @ 5 C	67.1% after 100 cycles @C/2	2.3 ~ 4.8	[35]
$LiNi_{0.9}Fe_{0.05}Mn_{0.05}O_2$	homogeneous co-precipitation and high-temperature solid-state	197.85 @ C/10, 194.89 @ C/5, 167.60 @ C/2	92.75% after 100 cycles @C/2	2.5 ~ 4.3	This work