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A Comprehensive Study of the Multiple Effects of Y/Al Substitution on O3-Type $NaNi_{0.33}Mn_{0.33}Fe_{0.33}O_2$ with Improved Cycling Stability and Rate Capability for Na-ion Battery Applications

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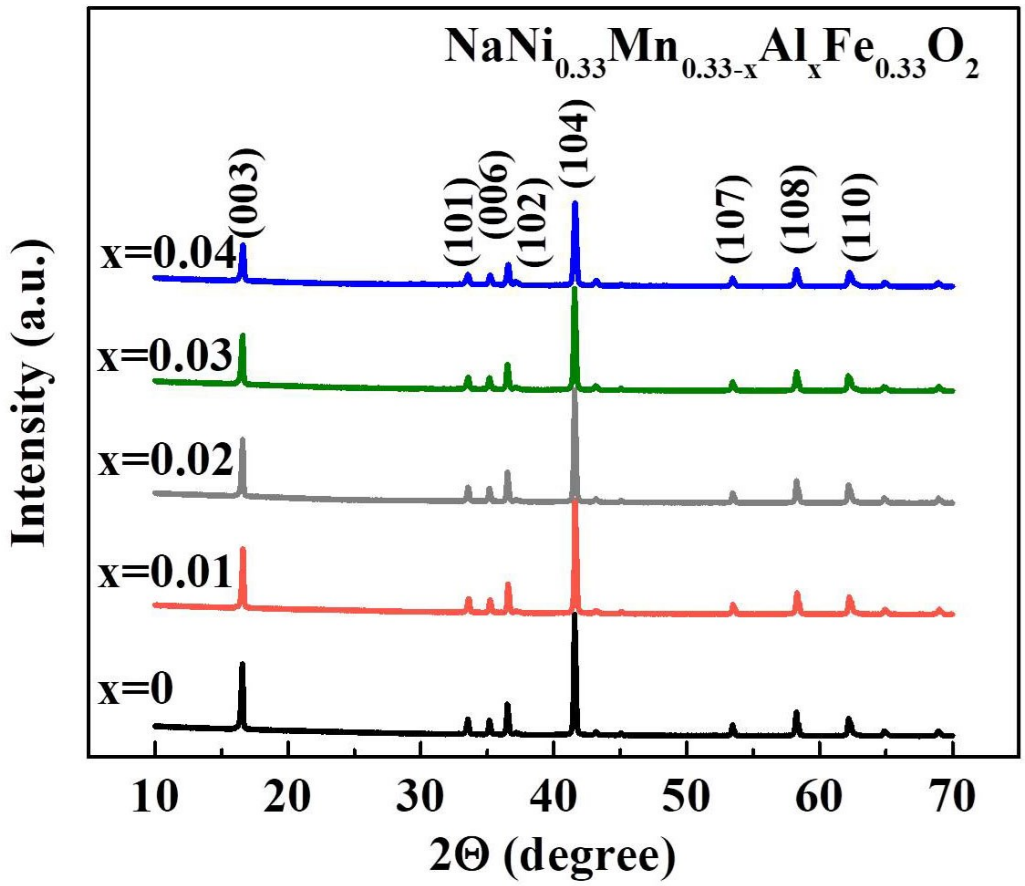

Figure S1. The X-ray diffraction patterns for Al-doped samples.

Table S1 Refined crystallographic lattice parameters of the $NaNi_{0.33}Mn_{0.33-x}Fe_{0.33}Y_xO_2$ samples.

Sample	pristine	Y0.01-doped	Y0.02-doped	Y0.03-doped	Y0.04-doped
Space group	$R\bar{3}m$	$R\bar{3}m$	$R\bar{3}m$	$R\bar{3}m$	$R\bar{3}m$
a (Å)	2.9791	2.9796	2.9810	2.9809	2.9806
c (Å)	16.0090	16.0129	16.0332	16.0326	16.0148
V (Å^3)	123.05	123.12	123.39	123.38	123.22
d-spacing (Å)	3.219	3.220	3.236	3.225	3.223
TMO2 (Å)	2.117	2.117	2.108	2.120	2.119
R_{wp} (%)	5.97	4.27	5.47	4.72	4.25
R_p (%)	3.75	2.68	3.24	2.75	2.70

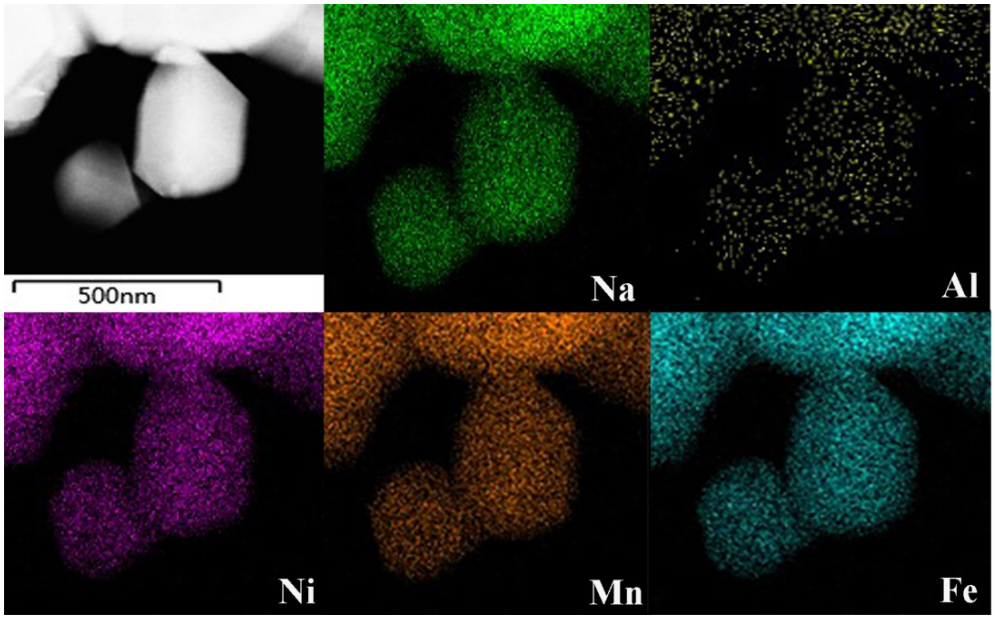

Figure S2. Elemental mapping images of the Al0.04-doped sample.

Table S2 The simulation results of EIS before cycling.

Samples	R_s		R_{ct}	
	Value(Ω)	Error%	Value(Ω)	Error%
$NaNi_{0.33}Mn_{0.33}Fe_{0.33}O_2$	20.61	2.52	653.33	2.02
$NaNi_{0.33}Mn_{0.31}Y_{0.02}Fe_{0.33}O_2$	13.96	2.31	300.63	1.79

Table S3 The simulation results of EIS after cycling.

Samples	R_s		R_{ct}	
	Value(Ω)	Error%	Value(Ω)	Error%
$NaNi_{0.33}Mn_{0.33}Fe_{0.33}O_2$	21.67	4.43	975.07	1.92
$NaNi_{0.33}Mn_{0.31}Y_{0.02}Fe_{0.33}O_2$	14.38	3.05	342.89	1.43

Table S4 The contents of lattice oxygen and surface oxygen in the cathode materials.

Samples	pristine	Y0.02-doped
Surface oxygen	68.96%	62.26%
Lattice oxygen	31.04%	37.74%