

Understanding the effect of Zn doping on stability of cobalt-free P2- $\text{Na}_{0.60}\text{Fe}_{0.5}\text{Mn}_{0.5}\text{O}_2$ cathode for Sodium Ion Batteries

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Table S1. Refined crystal sites and atom occupancies of $\text{Na}_{0.6}\text{Fe}_{0.5}\text{Mn}_{0.5}\text{O}_2$ (Zn-0) as determined by the Rietveld refinement.

Element	x	y	z	Wyckoff sites	Occupancy
Na1	0	0	0.25	2b	0.22
Na2	0.666667	0.333333	0.25	2d	0.38
Fe	0	0	0	2a	0.5
Mn	0	0	0	2a	0.5
O	0.333333	0.666667	0.093481	4f	1

Table S2. Refined crystal sites and atom occupancies of $\text{Na}_{0.6}\text{Fe}_{0.5}\text{Mn}_{0.49}\text{Zn}_{0.01}\text{O}_2$ (Zn-1) as determined by the Rietveld refinement.

Element	x	y	z	Wyckoff sites	Occupancy
Na1	0	0	0.25	2b	0.221
Na2	0.666667	0.333333	0.25	2d	0.379
Fe	0	0	0	2a	0.5
Mn	0	0	0	2a	0.49
O	0.333333	0.666667	0.097563	4f	1
Zn	0	0	0	2a	0.01

Table S3. Refined crystal sites and atom occupancies of $\text{Na}_{0.6}\text{Fe}_{0.5}\text{Mn}_{0.42}\text{Zn}_{0.02}\text{O}_2$ (Zn-2) as determined by the Rietveld refinement.

Element	x	y	z	Wyckoff sites	Occupancy
Na1	0	0	0.25	2b	0.203
Na2	0.666667	0.333333	0.25	2d	0.356
Fe	0	0	0	2a	0.5
Mn	0	0	0	2a	0.48
O	0.333333	0.666667	0.099382	4f	1
Zn	0	0	0	2a	0.02