

Supporting Information

A comprehensive picture of the current rate dependence on the structural evolution of **P2-Na_{2/3}Fe_{2/3}Mn_{1/3}O₂**

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Table S1. Cell 2, the electrode structure at the same state of charge (initial potential 2.86 V and in the 2nd cycle at 2.86 V). Na_{0.637(10)}Fe_{2/3}Mn_{1/3}O₂, the initial electrode and in bold Na_{0.66(10)}Fe_{2/3}Mn_{1/3}O₂ at the same potential during 2nd charge.

Atom	Wyckoff	X	Y	Z	SOF	Isotropic ADP (×100)/Å ²
Na(1)	2	0	0	0.25	0.171(7) 0.222(7)	3.55*
Na(2)	2	1/3	2/3	0.75	0.466(7) 0.436(8)	1.84*
Mn	2	0	0	0	1/3	2.68*,#
Fe	2	0	0	0	2/3	2.68*,#
O	4	1/3	2/3	0.0914(5) 0.0967(6)	1	4.10*

Atomic displacement parameter (ADP), site occupancy factor (SOF). *Refined alternatively to SOFs and refined and fixed. # Constrained to be equal. Spacegroup = *P6₃/mmc*, 23 refinement parameters, $\chi^2 = 3.1$, $R_p = 4.75\%$, $wR_p = 8.73\%$, $a = 2.95916(3)$, $c = 11.1489(1)$ Å. Spacegroup = *P6₃/mmc*, 23 refinement parameters, $\chi^2 = 3.33$, $R_p = 5.36\%$, $wR_p = 8.73\%$, $a = 2.94454(4)$, $c = 11.2231(1)$ Å.

Table S2. Refined crystallographic parameters for $\text{Na}_{0.326(12)}\text{Fe}_{2/3}\text{Mn}_{1/3}\text{O}_2$, cell 2 at the charged state.

Atom	Wyckoff	X	Y	Z	SOF	Isotropic ADP ($\times 100$)/ $\text{\AA}^2$
Na(1)	2	0	0	0.25	0.152(8)	3.55*
Na(2)	2	1/3	2/3	0.75	0.174(9)	1.84*
Mn	2	0	0	0	1/3	2.68* [#]
Fe	2	0	0	0	2/3	2.68* [#]
O	4	1/3	2/3	0.0876(6)	1	4.10*

Atomic displacement parameter (ADP), site occupancy factor (SOF). *Refined alternatively to SOFs and refined and fixed. # Constrained to be equal. Spacegroup = $P6_3/mmc$, 23 refinement parameters, $\chi^2 = 3.37$, $R_p = 5.37\%$, $wR_p = 9.61\%$, $a = 2.91455(4)$, $c = 11.4083(1)$ $\text{\AA}$.

Figure S1. The Fourier difference maps of the final model to the initial synchrotron XRD dataset of cell 2. The observed positive intensities are relatively weak. Left shows a higher cutoff intensity and right a lower cutoff intensity. Purple octahedral represent $\text{Fe}_{2/3}\text{Mn}_{1/3}\text{O}_6$ with oxygen in red, yellow and white spheres represent sodium with the proportion of yellow indicating sodium occupancy and the yellow non-spherical objects illustrating positive Fourier intensities.

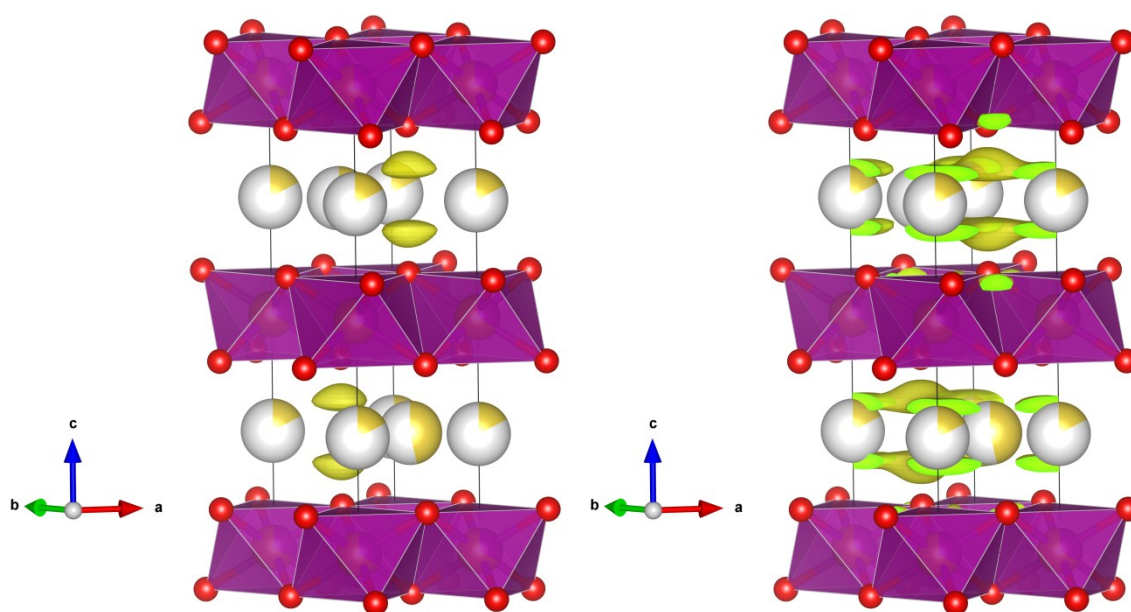


Figure S2. Rate performance of the P2 electrode charge and discharged at C/2.5 and 1C rates in conventional cells.

