Electronic Supplementary Material (ESI) for CrystEngComm.

Supplementary information

K modified P2-$Na_{0.7}Mn_{0.8}Mg_{0.2}O_2$ as a cathode material for sodium-ion batteries

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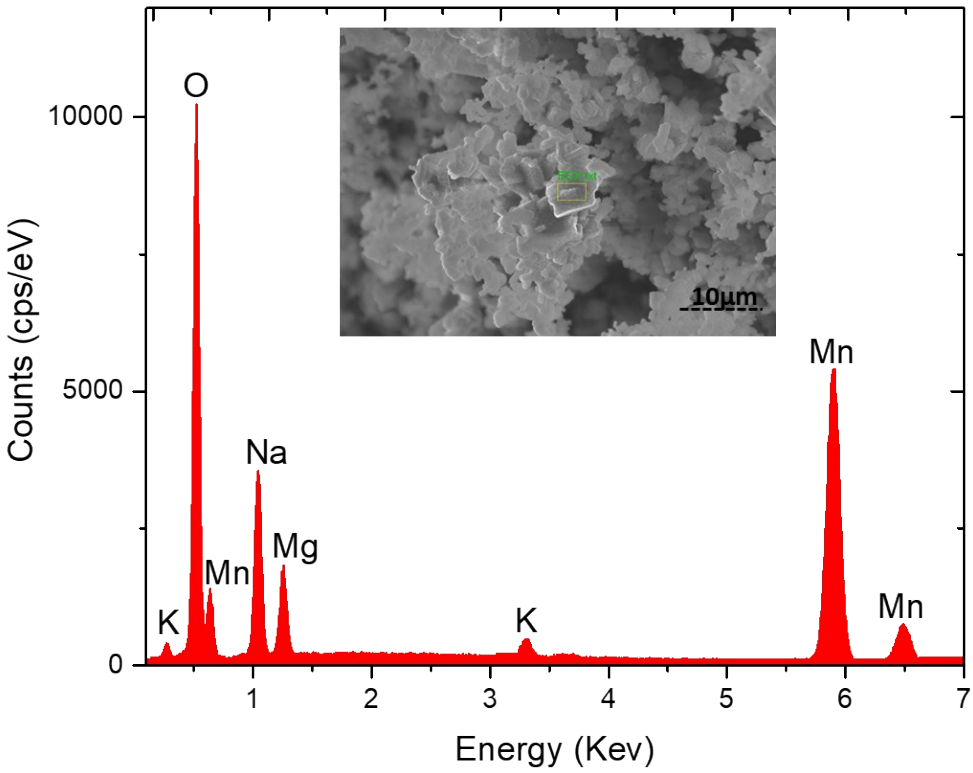

Fig. S1 EDS spectra on a selected area (rectangular region) of K-modified P2 $Na_{0.7}Mn_{0.8}Mg_{0.2}O_2$. SEM image is shown, on which EDX spectra was measured.

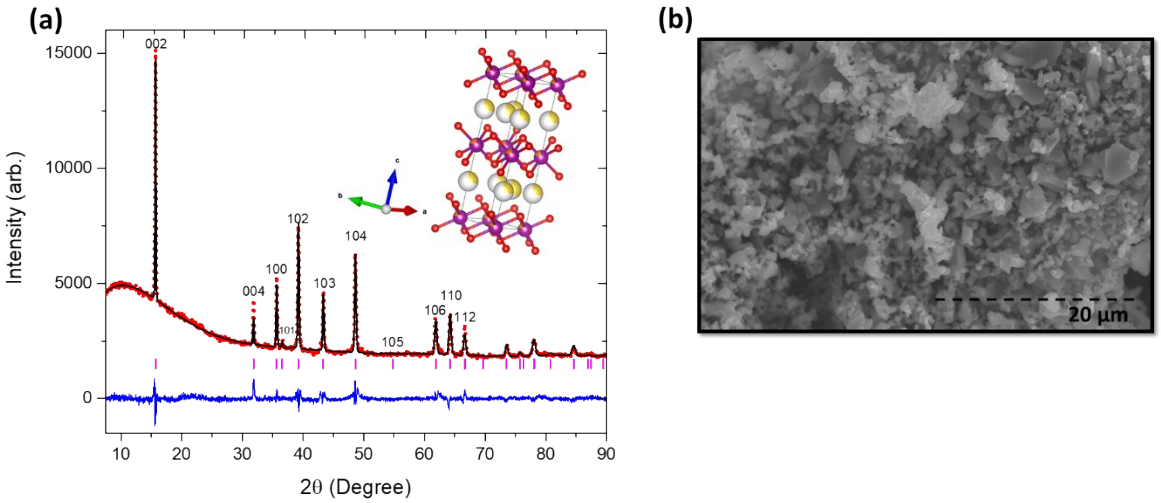

Fig. S2 (a) Rietveld refined fit of the $Na_{0.7}Mn_{0.8}Mg_{0.2}O_2$ structural model to the XRD data. Data are shown as red dots, the calculated Rietveld model as a line through the data, and the difference between the data and the model as the line below the data. The crystal structure of the materials with Mn in purple, O in red, Mg in orange, Na indicated by the amount of shading in yellow. **(b)** SEM images of P2 $Na_{0.7}Mn_{0.8}Mg_{0.2}O_2$ at 20 µm magnification.

Table S1. Crystallographic details of P2 $Na_{0.7}Mn_{0.8}Mg_{0.2}O_2$.

Name	*x* (*a*)	*y* (*b*)	z (*c*)	ADP (100 Å²)	SOF#
Mn	0	0	0	1.2(1)	0.8*
Mg	0	0	0	1.2(1)	0.2*
O	0.3333	0.6666	0.0931(2)	3.1(2)	1
Na_f	0.3333	0.6666	0.75	1.5^	0.4
Na_e	0	0	0.25	6.8^	0.3

ADP = atomic displacement parameter, SOF = site occupation factors, # = fixed, ^ refined initially then fixed, * constrained to be equal, nominal composition $Na_{0.7}Mn_{0.8}Mg_{0.2}O_2$, hexagonal $P6_3/mmc$ symmetry with lattice parameters a = 2.8918(2) Å and c = 11.181(1) Å, χ^2 = 1.05 wR_p = 3.58 %, 23 refinement parameters

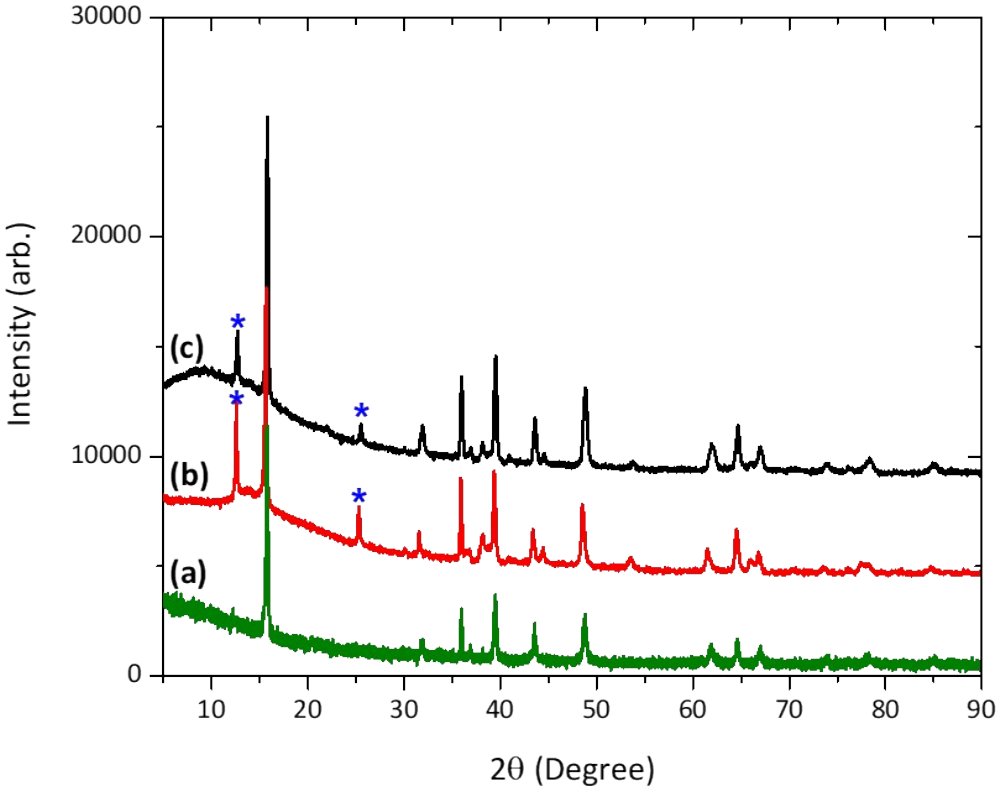

Fig. S3 XRD pattern of **(a)** sample quenched at 900 °C after heating for 12 hours and stored in Ar-filled glove box, **(b)** sample left outside the glove box for 2 days after quenching and **(c)** sample slow cooled to room temperature, after heating at 900 °C for 12 hours. Blue asterisks around ~12.4 and ~25.3° correspond to the (002) and (004) reflections of the hydrated P2 phase.

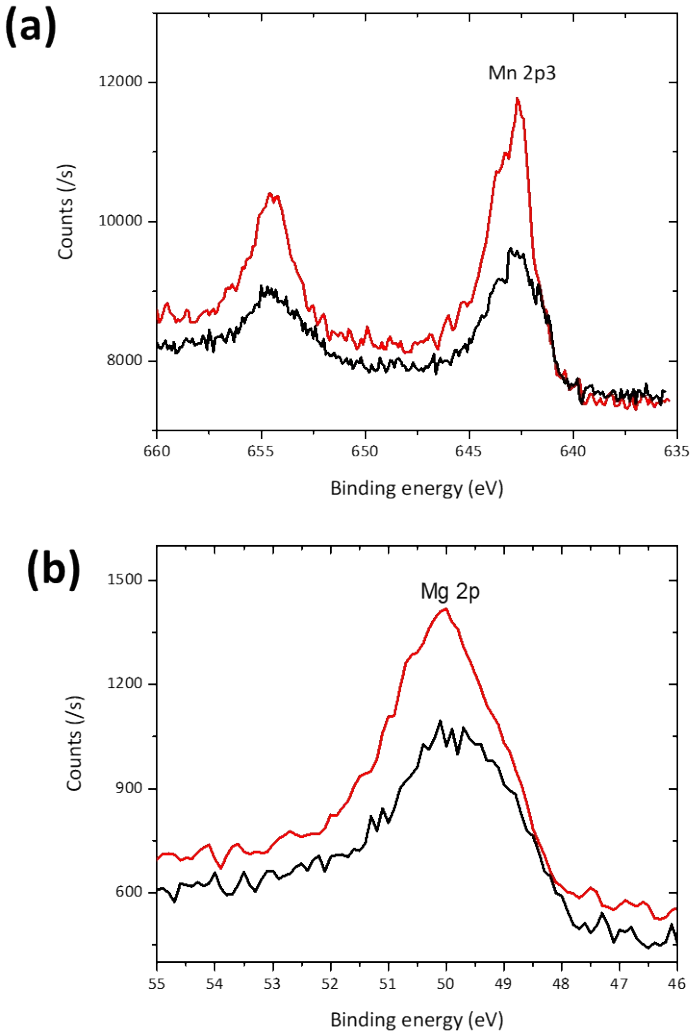

Fig. S4 XPS spectra of the $Na_{0.7}Mn_{0.8}Mg_{0.2}O_2$ (black) and K modified $Na_{0.7}Mn_{0.8}Mg_{0.2}O_2$ (red) electrode in the (a) Mn $2p^3$ and (b) Mg 2p regions.

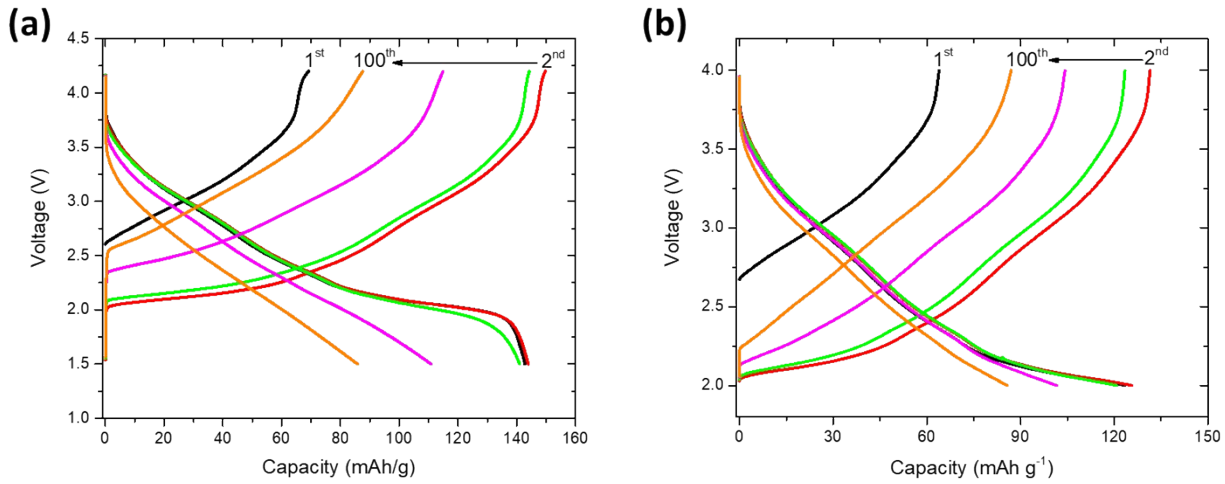

Fig. S5 Charge-discharge curves of P2 $Na_{0.7}Mn_{0.8}Mg_{0.2}O_2$ **(a)** between 1.5-4.2 V and **(b)** between 2-4 V at a current density of 15 mA g^{-1}. Black shows 1st, red 2nd, green 10th, pink 50th and orange 100th cycle.

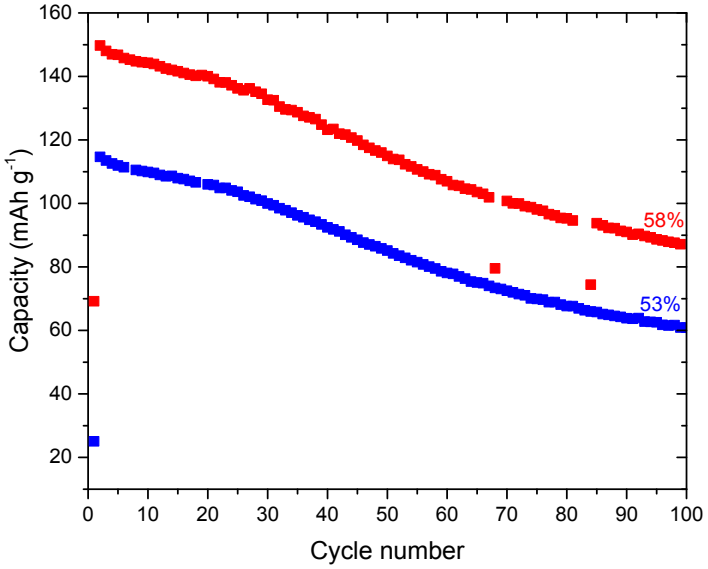

Fig. S6 Comparison of capacity retention curve of P2 $Na_{0.7}Mn_{0.8}Mg_{0.2}O_2$ (red square) and K-modified $Na_{0.7}Mn_{0.8}Mg_{0.2}O_2$ (blue square) between 1.5- 4.2 V at a current density of 15 mA g^{-1}.

Table S2. ICP results of K-modified P2 $Na_{0.7}Mn_{0.8}Mg_{0.2}O_2$.

Ratio	Expected	As found in synthesised powder	On separator after 1st charge to 4.2 V	On separator after 1st discharge to 1.5 V
K: Na	0.1428	0.10	0.066	0.048