Structure-electrochemical evolution of a Mn-rich P2 $Na_{2/3}Fe_{0.2}Mn_{0.8}O_2$ Na-ion battery cathode

Wesley M. Dose[1], Neeraj Sharma[2,*], James C. Pramudita[2,3], Helen E. A. Brand[4], Elena Gonzalo[5], Teofilo Rojo[5,6,*]

[1] Chemical Sciences and Engineering (CSE) Division, Argonne National Laboratory, Argonne, Illinois, U.S.A. 60439
[2] School of Chemistry, UNSW Sydney, Sydney NSW 2052, Australia
[3] Australian Centre for Neutron Scattering, Australia Nuclear Science and Technology Organisation, Kirrawee, DC NSW 2253, Australia
[4] Australian Synchrotron, 800 Blackburn Road, Clayton VIC 3168, Australia
[5] CICenergigune, Parque Tecnológico de Álava, Albert Einstein 48, ED.CIC, 01510, Miñano, Spain
[6] Departamento de Química Inorgánica, Universidad del País Vasco UPV/EHU, P.O. Box. 644, 48080, Bilbao, Spain

Supporting Information

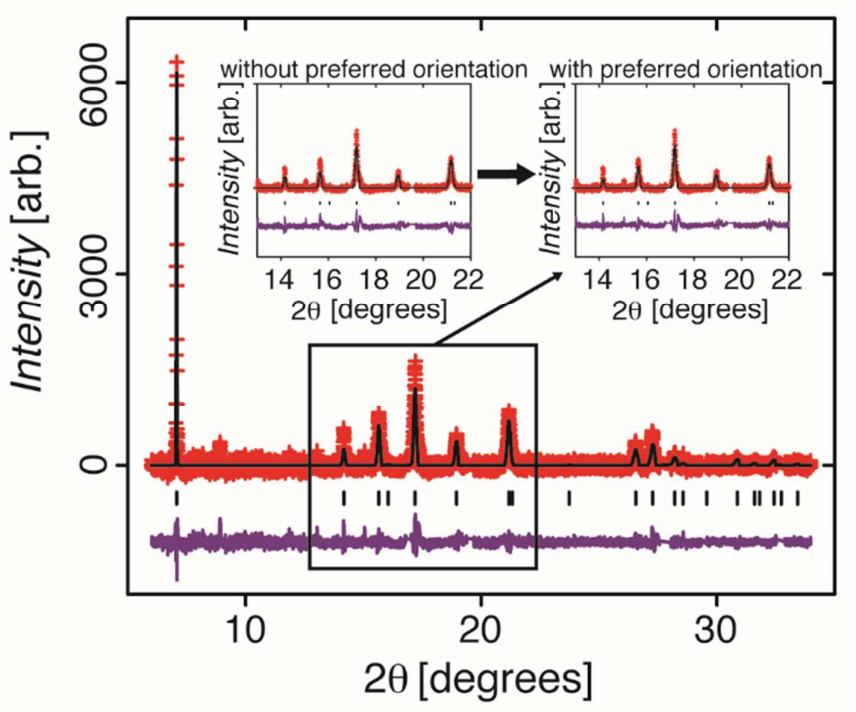

Figure [S1]. Rietveld refined fit of the $Na_{0.74(2)}Fe_{0.2}Mn_{0.8}O_2$ model to the initial *in situ* synchrotron XRD dataset, with a 100 preferred orientation term (March-Dollase). Data are shown as crosses, the calculated Rietveld model as a line through the data, and the difference between the data and the model as the line below the data. The vertical reflection markers are for P2 $Na_{0.74(2)}Fe_{0.2}Mn_{0.8}O_2$. The insert shows the fit in the region $13 \leq 2\theta \leq 22$ without (left) and with (right) the 100 preferred orientation term.

Table S1. Refined crystallographic parameters for $Na_{0.74(2)}Fe_{0.2}Mn_{0.8}O_2$.

Atom	Wyckoff	x	y	z	SOF[a)]	Isotropic ADP[a)] (×100 Å²)
Na_f	2	0	0	0.25	0.26(1)	6.7*
Na_e	2	1/3	2/3	0.75	0.48(1)	2.2*
Mn	2	0	0	0	0.8	2.9*,#
Fe	2	0	0	0	0.2	2.9*,#
O	4	1/3	2/3	0.0958(8)	1	4.3*

[a)] Atomic displacement parameter (ADP), site occupancy factor (SOF). * Refined alternatively to SOFs and refined and fixed. # Constrained to be equal. Space group $P6_3/mmc$, 31 refinement parameters, χ^2 = 1.95, R_p = 3.02 %, wR_p = 4.10 %, a = 2.9176(1) Å, c = 11.1589(2) Å.