

Layered P2-O3 sodium-ion cathodes derived from earth abundant elements

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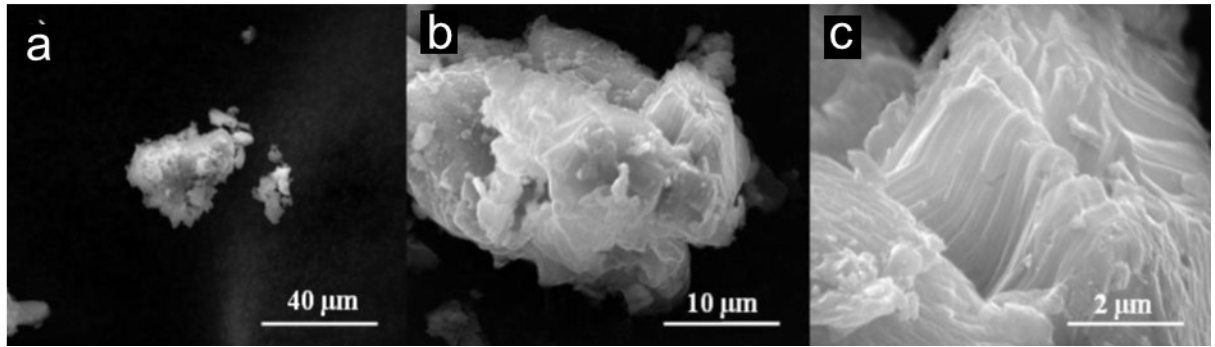


Figure S1. SEM images of the synthesized P2/O3 material at different magnifications.

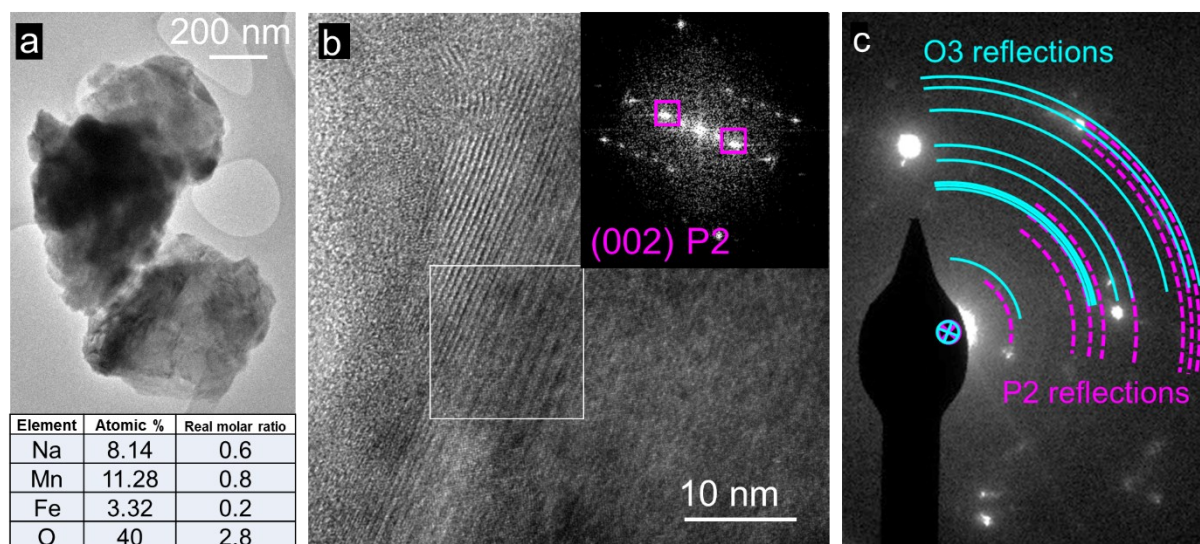


Figure S2. (a) Low magnification TEM image of a particle and related Energy-dispersive X-ray spectroscopy (EDX) analysis showing a good agreement with the theoretical composition; (b) High resolution TEM image and the local FFT image in the inset showing the P2 (002). (c) Local SAED pattern of the selected particle, the arcs indicate the expected positions for the P2 and O3 reflections.

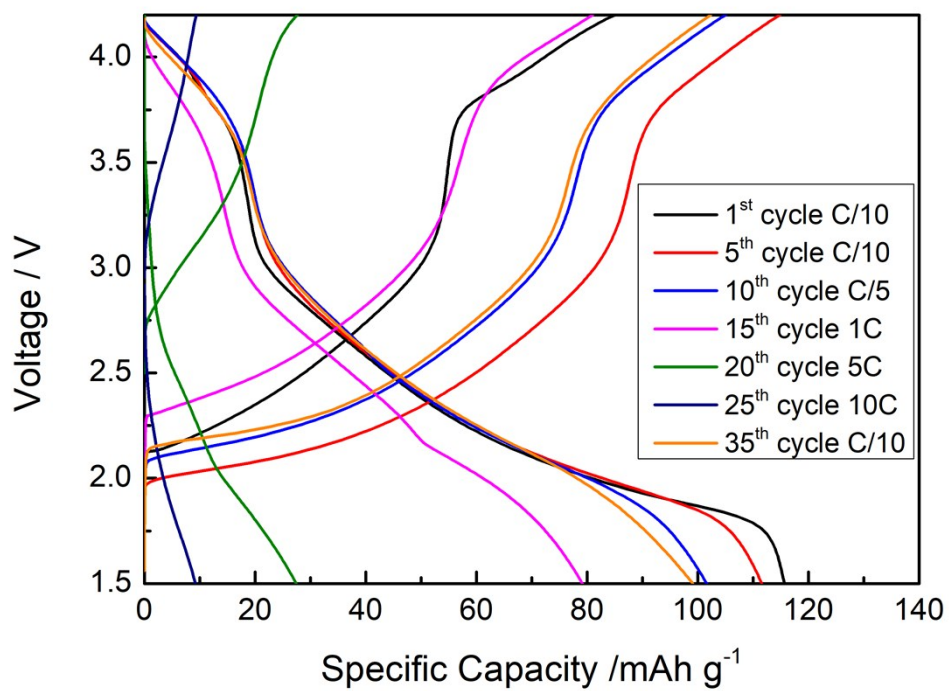


Figure S3. Voltage profiles of the P2/O3-material cycled at various C rates between 1.5 and 4.2 V vs. Na⁺/Na.

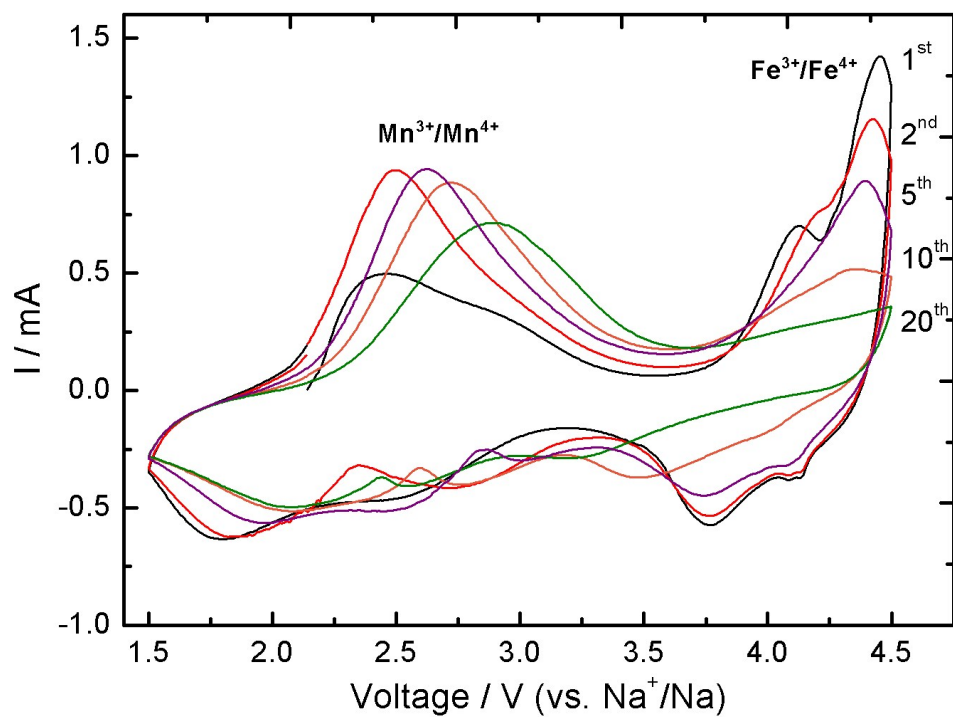


Figure S4. Cyclic voltammogram profiles of pristine sample, active mass 2.42 mg at a scan rate of 1 mV s⁻¹

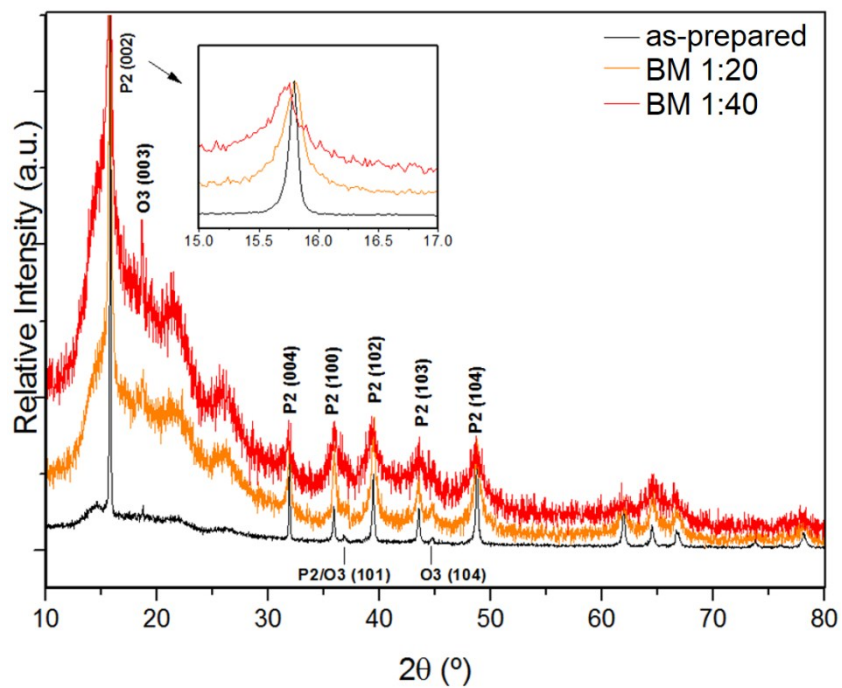


Figure S5. PXRD patterns normalized to the intensity of the pristine sample and after ball milling with different powder-to-ball ratio: 1:20 (orange curve) and 1:40 (red curve).

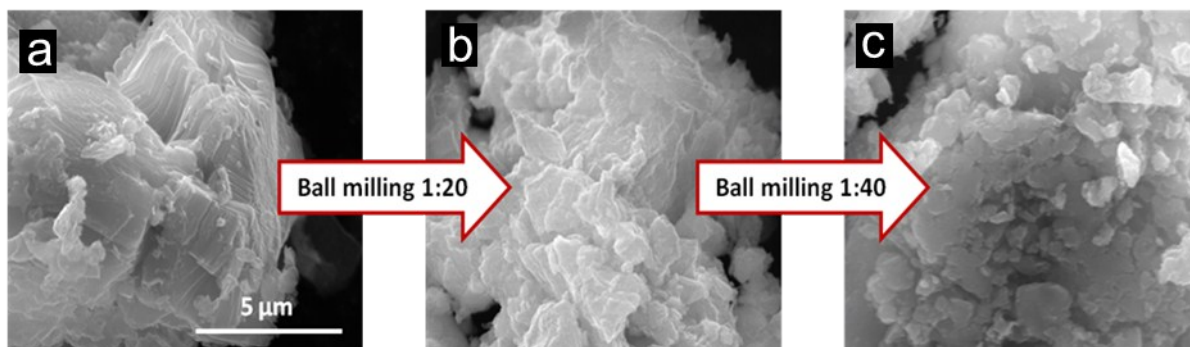


Figure S6. SEM images at magnification of 20000X of (a) as-prepared, and ball milled samples at (b) 1:20 and (c) 1:40 powder-to-ball ratios.

Table 1. Refined values of the lattice parameters and agreement factors for the pristine material, together with the refined atomic positions and occupancy (SOF) obtained by FullProf software^[37] for the P2 phase.

Phase	a, b (Å)	c (Å)	χ^2	Rp; Rwp; Rexp	
P2	2.888(2)	11.20(2)	2.25	4.51; 6.48; 4.58	
O3	2.84(2)	14.2(1)			
Atom	Wyckoff	x	y	z	SOF
Na1	2	0	0	¼	0.141(6)
Na2	2	1/3	2/3	¾	0.419(7)
Li	2	0	0	¼	0.18
Mn	2	0	0	0	0.80
Fe	2	0	0	0	0.167(7)
O	4	1/3	2/3	0.077(8)	2

Table 2. Concentration (in ppm) of the experimental and theoretical molar ratio (fixing Mn content) of the elements detected in the sample by ICP-OES measurement.

Element	ICP Concentration (ppm)	Experimental molar ratio	Theoretical molar ratio
Na	6.61	0.62	0.67
Mn	20.4	0.8	0.8
Fe	4.82	0.19	0.2
Li	0.574	0.18	0.18

Table 3. Lattice parameters and agreement factors for the pattern recorded at OCV, 4.2 V and 1.5 V. The pattern matching was performed using FullProf software.^[37]

Voltage	P2		O3		P2			χ^2	Rp; Rwp; Rexp
	a, b (Å)	c (Å)	a, b (Å)	c (Å)	a (Å)	b (Å)	c (Å)		
OCV	2.887(4)	11.20(1)	2.848(5)	14.20(6)				2.79	5.73; 7.75; 4.64
4.2V	2.865(7)	11.27(1)	2.84(2)	14.20(8)				2.3	4.77; 7.04; 4.64
1.5V	2.93(1)	10.99(2)	2.848(5)	14.22(7)	2.86(2)	5.35(4)	10.81(1)	1.95	5.35; 6.92; 4.95