Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

Aliovalent-doped sodium chromium oxide ($Na_{0.9}Cr_{0.9}Sn_{0.1}O_2$ and $Na_{0.8}Cr_{0.9}Sb_{0.1}O_2$) as sodium-ion battery cathodes with high-voltage characteristics

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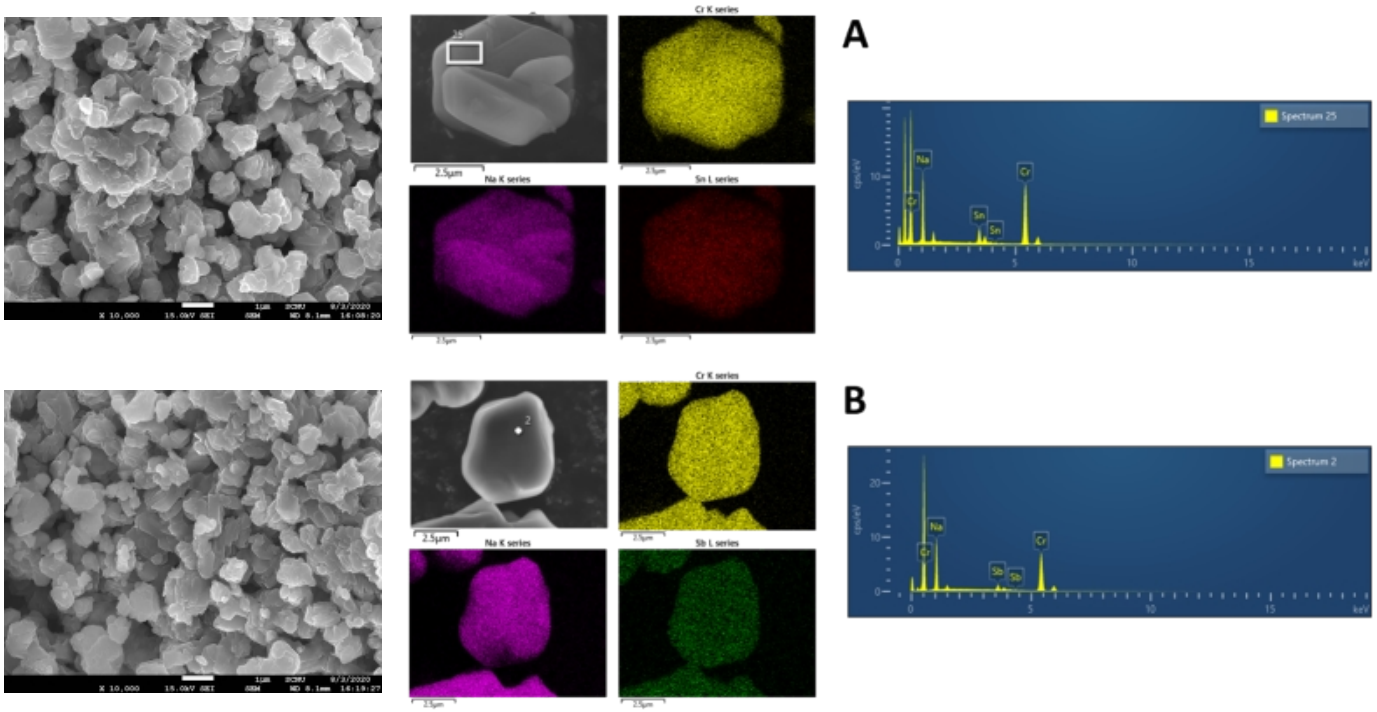

Fig. S1. FESEM and elemental mapping images with corresponding EDX spectra of (A) NCSnO and (B) NCSbO. EDX spectra indicate the composition of $Na_{0.89\pm0.02}Cr_{0.91\pm0.02}Sb_{0.09\pm0.01}O_2$ and $Na_{0.80\pm0.02}Cr_{0.91\pm0.02}Sb_{0.09\pm0.00}O_2$ for NCSnO and NCSbO, respectively,

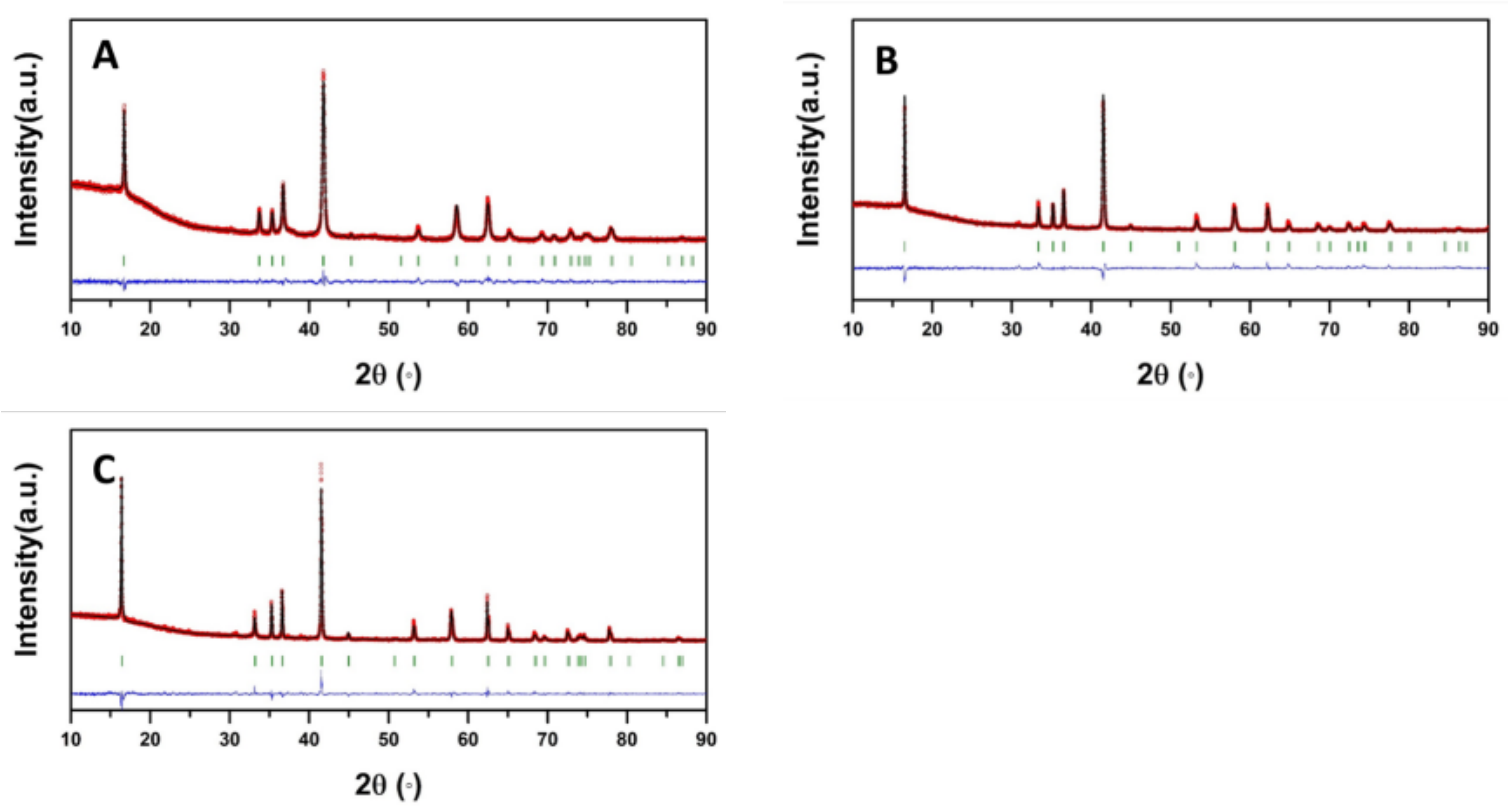

Fig. S2. Full-pattern Rietveld refinements of (A) NCO, (B) NCSnO, and (C) NCSbO. Experimental, calculated, and difference profiles are shown by the red dots, black line, and blue line, respectively. The green vertical tick marks above the difference profile denote the positions of Bragg reflections. For the best fit between the observed and calculated data, the profile shapes were defined using a pseudo-Voigt function. No preferred orientation was applied.

Table S1 Lattice parameters and atomic coordinates of a P'3 phase ($Na_{0.4}CrO_2$) in $Na_{0.3}CrO_2$.

Atom	Wyckoff symbol	x/a	y/b	z/c	U (Å²)	S.O.F.
Na	4i	0.202 (7)	0	0.553 (9)	0.004 (4)	0.2
Cr	2a	0	0	0	0.0057 (20)	1
O	4i	0.397 (9)	0	0.177 (2)	0.004 (16)	1
Space group: *C*2/m						
Number of formula per unit cell (z) = 2						
Lattice parameters: a = 4.990 (4) Å, b = 2.892 (2) Å, c = 5.902 (3) Å, α = γ = 90°, β = 106.60 (9)°						

Table S2 Lattice parameters and atomic coordinates of an O3' phase ($Na_{\delta}CrO_2$) in $Na_{0.3}CrO_2$.

Atom	Wyckoff symbol	x/a	y/b	z/c	U (Å²)	S.O.F.
Cr	3a	0	0	0	0.0036	0.667
Cr	6c	0	0	0.126 (2)	0.0121	0.167
O	6c	0	0	0.249 (4)	0.0108	1
Space group: *R*-3m						
Number of formula per unit cell (z) = 3						
Lattice parameters: a = 2.899 (1) Å, c = 13.905 (9) Å, α = β = 90°, γ = 120°						

Table S3 Lattice parameters and atomic coordinates of $Na_{0.4}[Cr_{0.9}Sn_{0.1}]O_2$.

Atom	Wyckoff symbol	x/a	y/b	z/c	U (Å²)	S.O.F.
Na	4i	0.252 (4)	0	0.499 (3)	0.037 (10)	0.2
Cr	2a	0	0	0	0.0003 (7)	0.9
Sn	2a	0	0	0	0.0003 (7)	0.1
O	4i	0.389 (4)	0	0.1735 (8)	0.0227 (18)	1.0
Space group: *C*2/m Number of formula per unit cell (z) = 2 Lattice parameters: a =5.0663 (4) Å, b = 2.9259 (2) Å, c = 5.9331 (2) Å, α = γ = 90°, β = 106.28 (1)°						

Table S4 Lattice parameters and atomic coordinates of $Na_{0.3}[Cr_{0.9}Sb_{0.1}]O_2$.

Atom	Wyckoff symbol	x/a	y/b	z/c	U (Å²)	S.O.F.
Na	4i	0.199 (8)	0	0.551 (4)	0.025 (7)	0.15
Cr	2a	0	0	0	0.0316 (8)	0.9
Sb	2a	0	0	0	0. 0316 (8)	0.1
O	4i	0.3808 (16)	0	0.1778 (8)	0.0122 (16)	1.0
Space group: *C*2/m Number of formula per unit cell (z) = 2 Lattice parameters: a =5.0313 (2) Å, b = 2.9110 (1) Å, c = 5.9457 (2) Å, α = γ = 90°, β = 106.75 (1)°						