Supporting Information

Development of a new alluaudite-based cathode material with high power and long cyclability for application of Na-ion batteries in real-life

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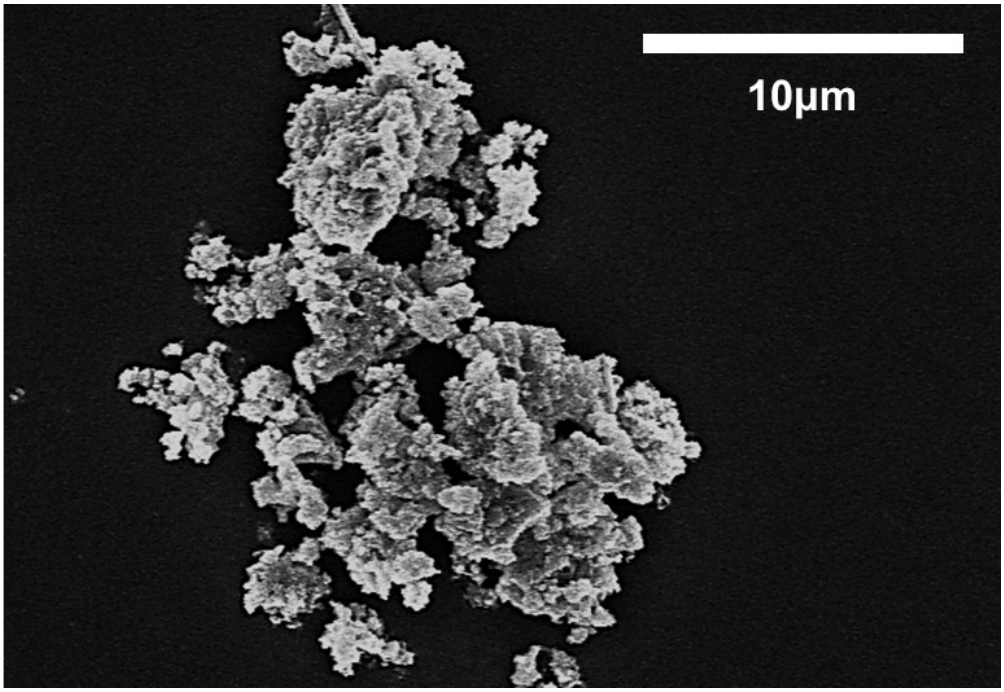
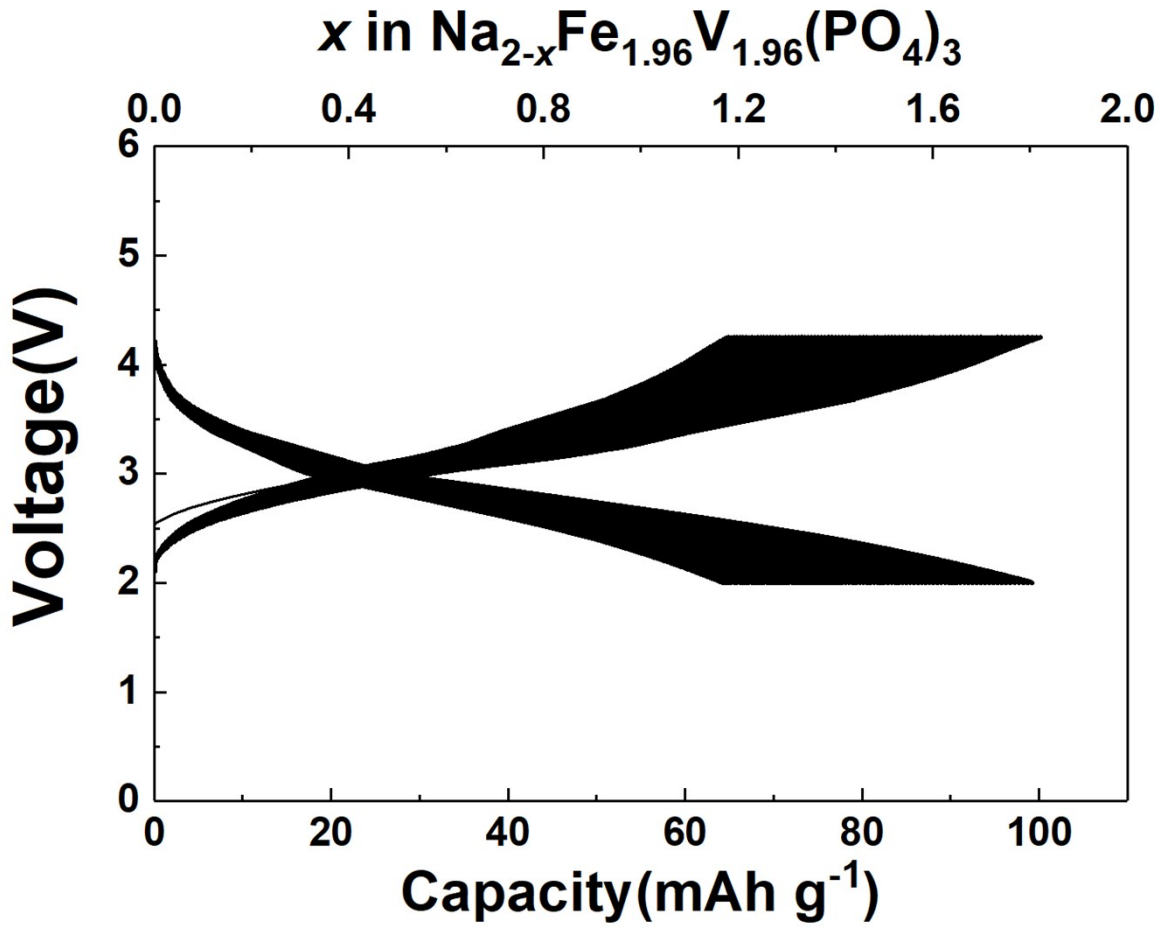
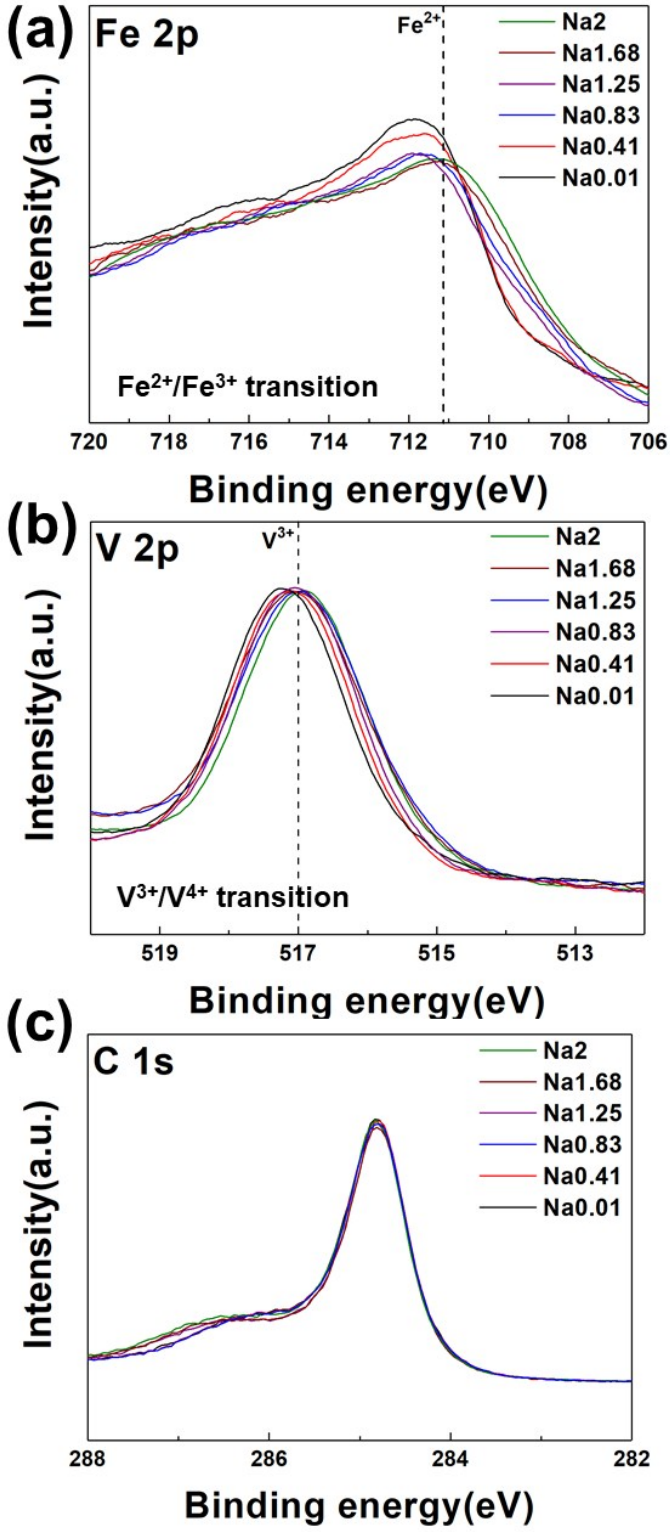


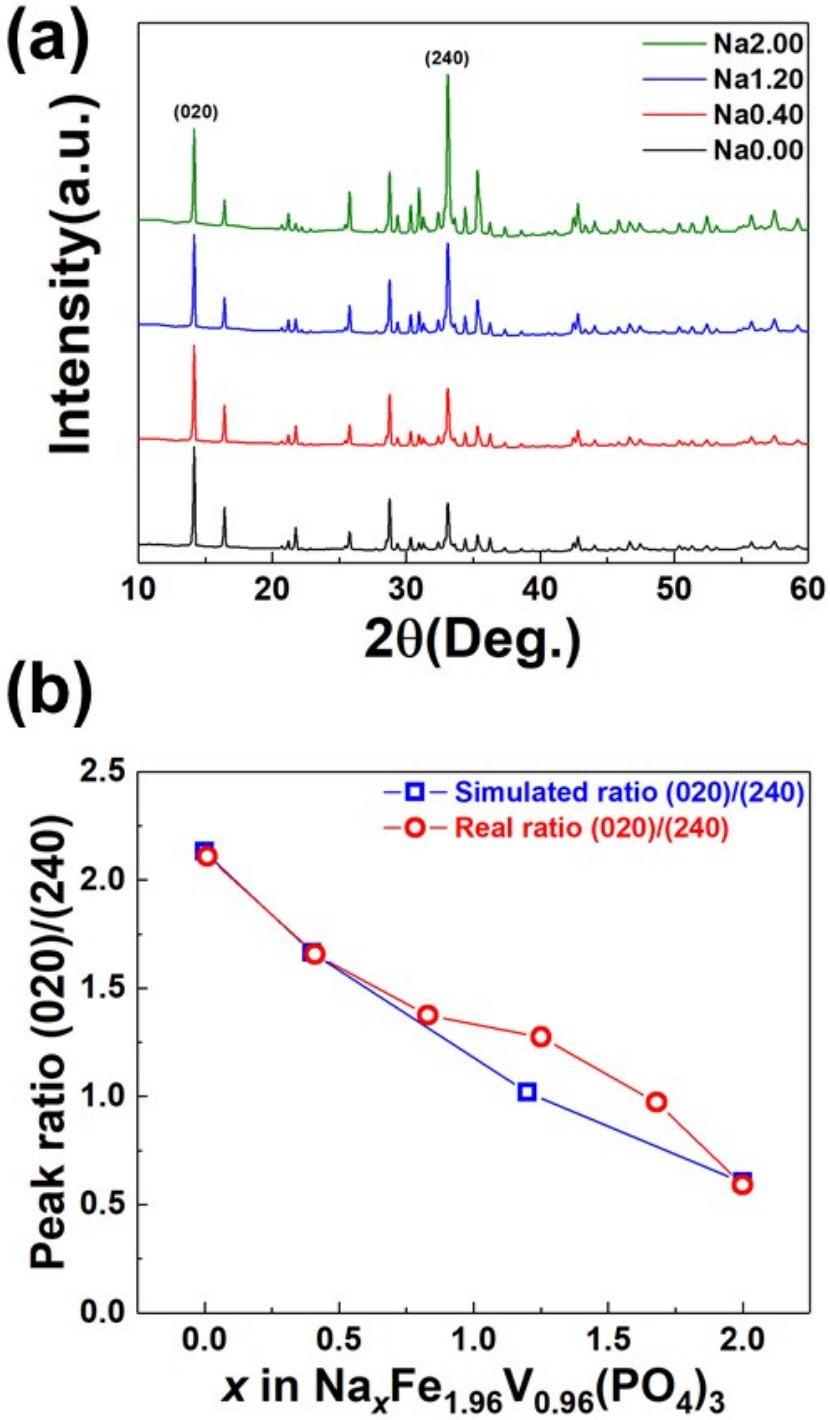
Supporting Figure S1. The SEM image of NFVP



Supporting Figure S2. Charge/discharge curves of NFVP over 2500 cycles at 1C.



Supporting Figure S3 *ex-situ* (a) Fe 2p, (b) V 2p, and C 1s XPS spectra of NFVP as function of Na amounts in the structure.



Supporting Figure S4 (a) Simulated X-ray diffraction pattern of various $Na_xFe_{1.96}V_{0.96}(PO_4)_3$ ($0 \leq x \leq 2$) and (b) Comparison of peak-intensity ratio of (020) and (240) between simulation data and real data.

Atom	Site	*x*	*y*	*z*	B_{iso}	Occupancy
Na1	4b	0	0.5	0	1.1(3)	1.000(6)
Na2	4e	0	-0.0116(15)	0.25	1.9(4)	0.922(6)
Fe1	4e	0	0.2698(6)	0.25	1.07(19)	0.998(3)
V1	4e	0	0.2698(6)	0.25	1.07(19)	0.002(2)
Na3	4e	0	0.2698(6)	0.25	1.07(19)	0.000(4)
Fe2	8f	0.2803(5)	0.6650(3)	0.3662(10)	0.80(12)	0.481(2)
V2	8f	0.2803(5)	0.6650(3)	0.3662(10)	0.80(12)	0.478(2)
Na4	8f	0.2803(5)	0.6650(3)	0.3662(10)	0.80(12)	0.041(5)
P1	4e	0	0.7136(10)	0.25	1.0(3)	1.00(2)
P2	8f	0.2331(8)	0.8908(5)	0.1200(16)	0.7(2)	1.00(3)
O1	8f	0.4503(11)	0.7138(11)	0.534(2)	0.4(4)	1
O2	8f	0.1034(14)	0.6354(9)	0.254(2)	0.8(4)	1
O3	8f	0.3417(11)	0.6608(11)	0.111(2)	0.7(4)	1
O4	8f	0.1282(12)	0.3975(8)	0.3297(18)	0.4(4)	1
O5	8f	0.2219(12)	0.8256(9)	0.307(2)	0.5(4)	1
O6	8f	0.3287(8)	0.5007(11)	0.3861(15)	0.8(3)	1

Calculated atomic composition: $Na_{1.92}Fe_{1.00}(Fe_{0.96}V_{0.96}Na_{0.08})(PO_4)_3 \rightarrow Na_{2.00}Fe_{1.96}V_{0.96}(PO_4)_3$

Supporting Table T1. The structural data on NFVP analyzed using simultaneous Rietveld refinement of the X-ray diffraction (XRD) and neutron diffraction (ND) patterns.