Supporting Information

$Na_{0.97}KFe(SO_4)_2$: New iron-based sulfate cathode material with outstanding cyclability and power-capability for Na-ion batteries

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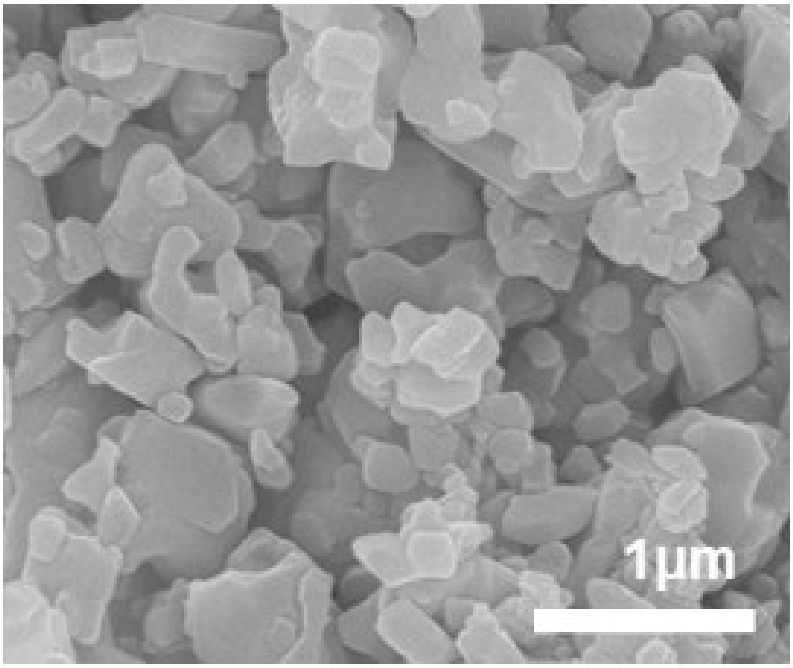
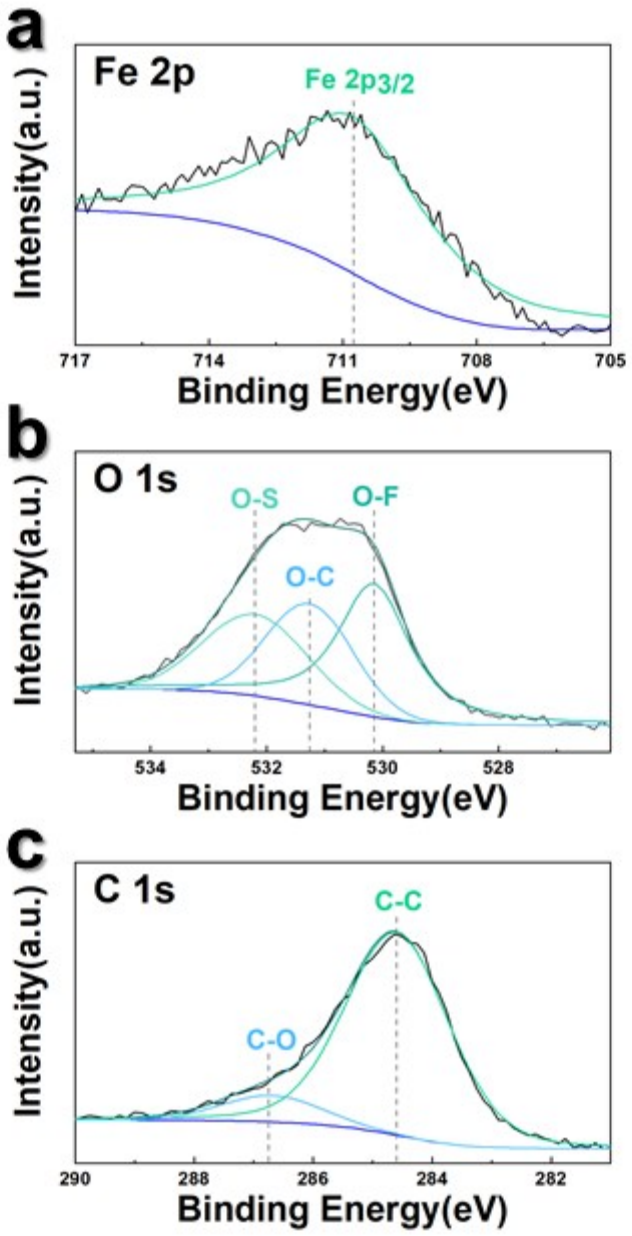
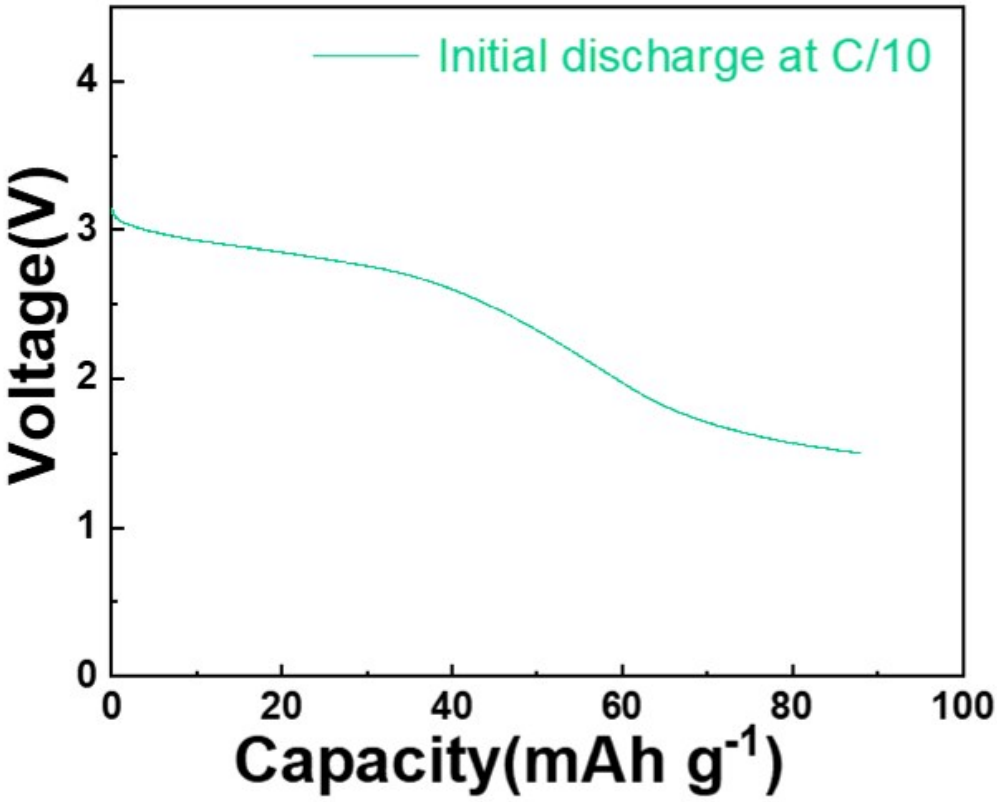


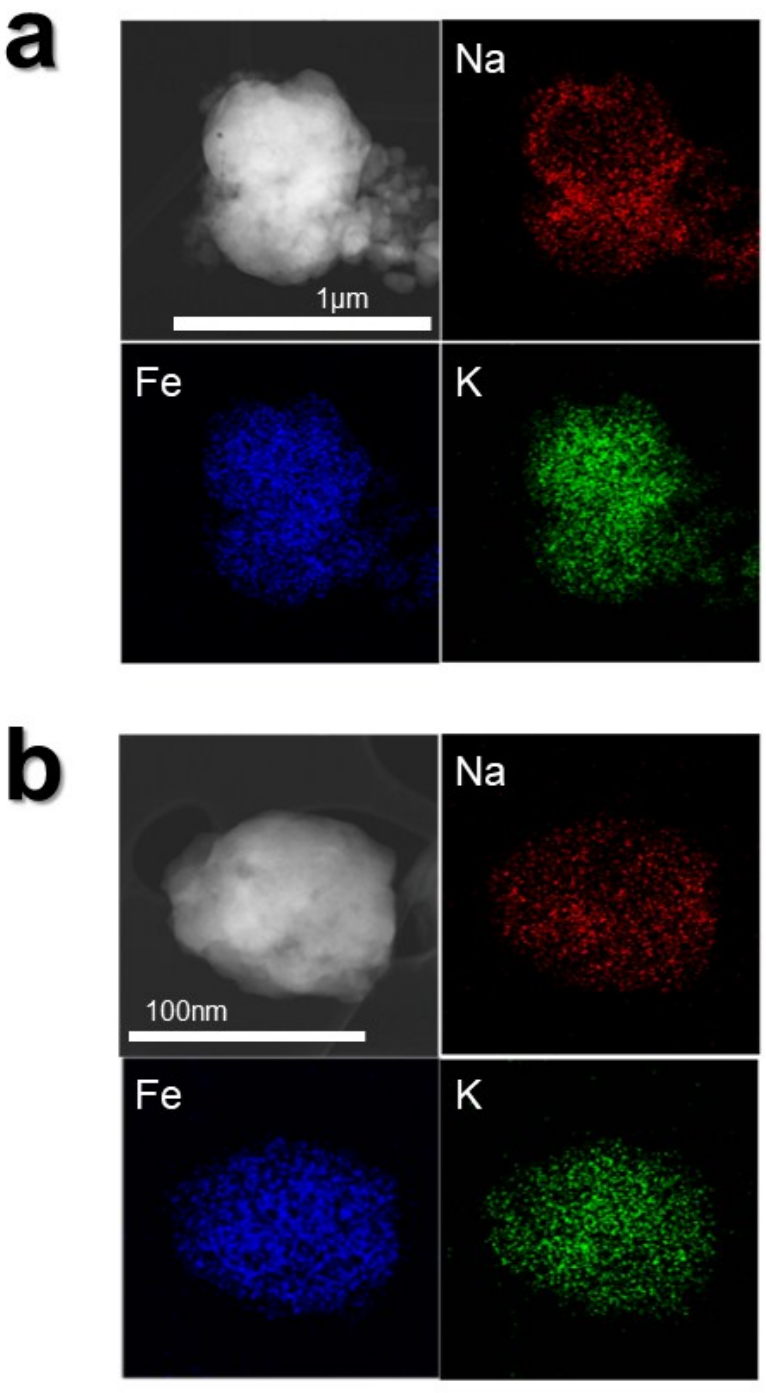
Supporting Figure S1. SEM image of bare $KFe(SO_4)_2$ powder.



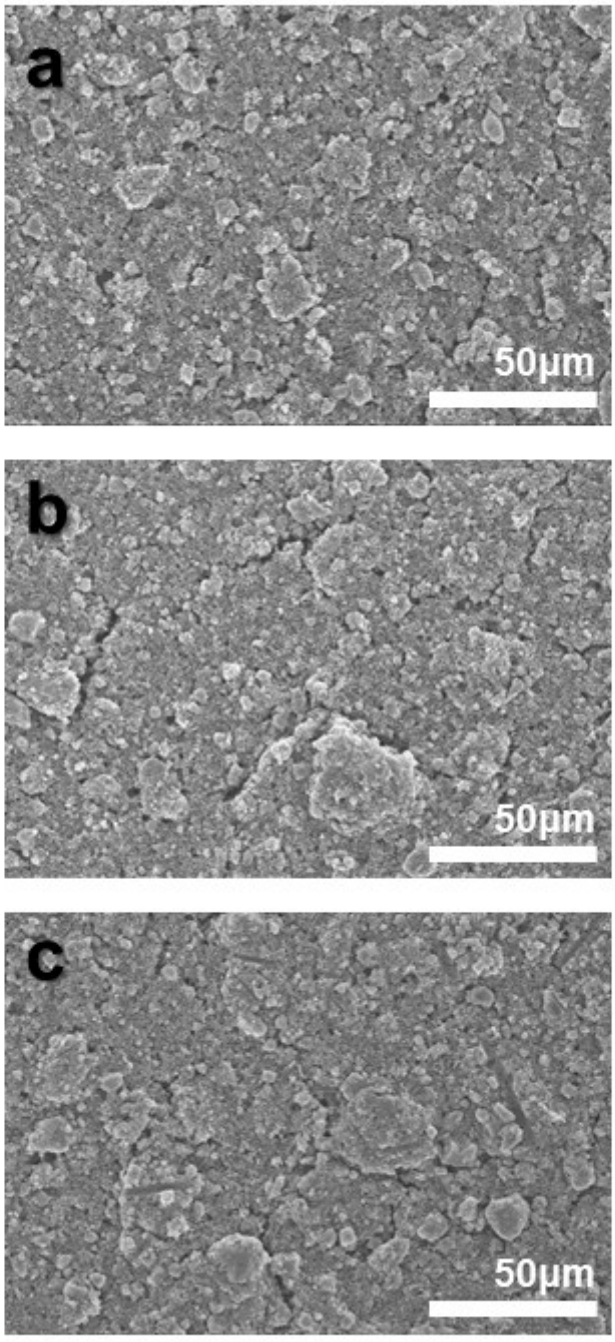
Supporting Figure S2. XPS spectra of $KFe(SO_4)_2$. (a) Fe 2p peak as Fe 2p3/2 (710.8eV)[1], (b) O 1s peaks as O-S (532.2eV)[2], O-F (~529.9eV)[2] and O-C(532.1eV)[3], (c) C 1s peaks as C-C (284.6eV)[4] and C-O (286.75eV)[5].



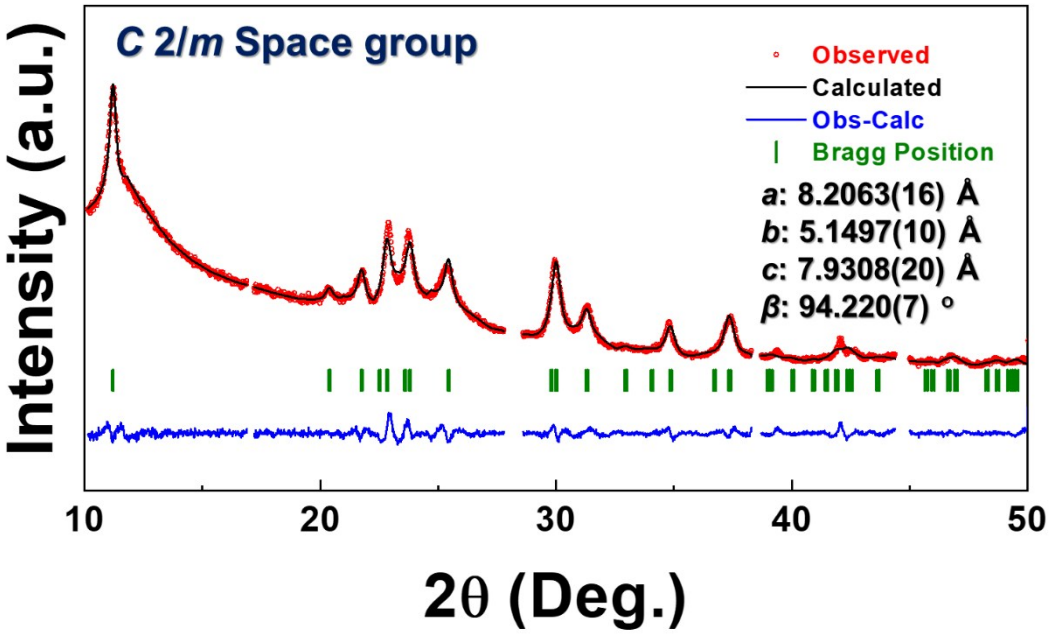
Supporting Figure S3 Initial discharge curve of $Na_{0.97}KFe(SO_4)_2$ measured at C/10



Supporting Figure S4 TEM EDS mapping of $Na_{0.97}KFe(SO_4)_2$ after (a) 200 cycles (atomic ratio of Na and K = 1.10 : 1) and (b) 2 cycles (atomic ratio of Na and K = 1.03 : 1).



Supporting Figure S5 SEM images of electrodes. (a) before cycling, (b) after 100 cycles, (c) after 200cycles.



Supporting Figure S6 Refined XRD pattern of after 200cycles $Na_0KFe(SO_4)_2$ (R_P = 2.47%, R_I = 1.81%, R_F = 1.25%, χ^2 = 2.02%)

Atom	Multiplicity	*x*	*y*	*z*	B_{iso}	Occupancy
Fe	2	0.00000	0.00000	0.00000	0.88(6)	1
K	2	0.00000	0.00000	0.50000	1.50(8)	1
S	4	0.3713(3)	0	0.2072(3)	0.79(7)	1
O1	4	0.2466(6)	0	0.0719(6)	0.73(8)	1
O2	4	0.3113(7)	0	0.3795(6)	0.73(8)	1
O3	8	0.4726(4)	0.2332(5)	0.1875(4)	0.73(8)	1

Supporting Table T1. The structural information of $KFe(SO_4)_2$ using Rietveld refinement calculation.

	Na	K	Fe
Pristine sample	0	0.988(6)	0.998(3)
Fully discharged sample	0.989(5)	0.981(7)	0.995(5)
200 times cycled sample	0.987(6)	0.982(5)	0.996(3)

Supporting Table T2 ICP analyses on the atomic ratio of Na, K, Fe in the pristine sample, the fully discharged sample and the 200 times cycled sample of $Na_{0.97}KFe(SO_4)_2$ with standard deviation.

References

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