Supporting Information for

P3-type Layered $K_{0.6}Cr_{0.6}Ti_{0.4}O_2$ for Potassium Storage Applications

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Supporting Table S1. Crystallographic parameters refined by Rietveld analysis of XRD data (λ = 1.5418 Å) of $K_{0.6}Cr_{0.6}Ti_{0.4}O_2$ at 25 ˚C.

Formula $K_{0.6}Cr_{0.6}Ti_{0.4}O_2$						
Space group *R*-3*m*						
a = 2.968 Å, c = 19.06 Å						
R_{wp} = 19.8%, R_B = 12.0%						
atom	site	*x*	*y*	*z*	*B* / Å²*	*g**
K	18*h*	0.10	-0.10	0.169	0.8	0.1
Cr	3*a*	0	0	0	0.5	0.6
Ti	3*a*	0	0	0	0.5	0.4
O	6*c*	0	0	0.377	1.0	1.0

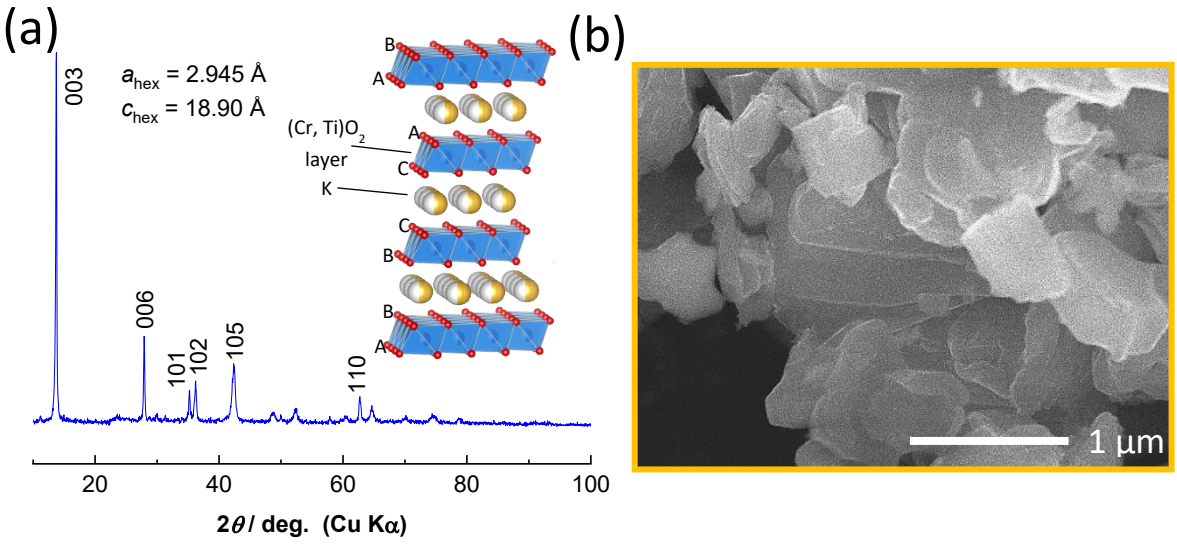
* Not refined

Supporting Table S2. Unit cell volume changes of some reported K-based layered positive electrodes.

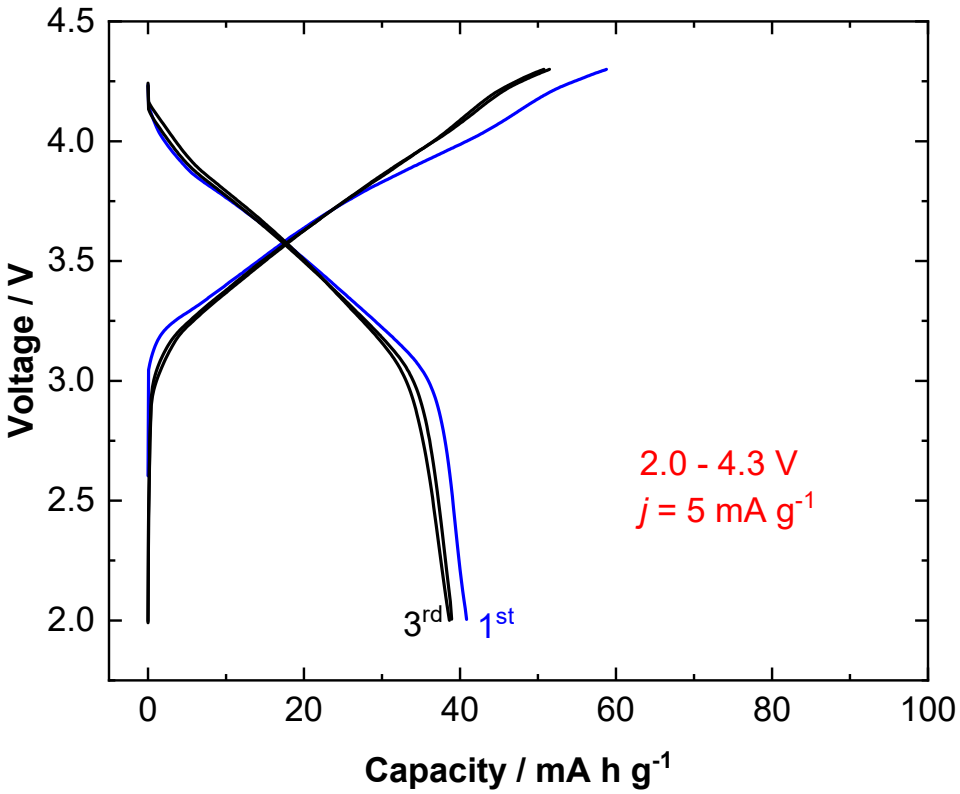
Composition	Volume change upon charge/discharge (%)	Reference
$K_{0.67}MnO_2$	9.9	1
$K_{0.75}[Ni_{1/3}Mn_{2/3}]O_2$	3.1	2
$K_{0.3}Mn_{0.95}Co_{0.05}O_2$	2.5	3
$K_{0.3}MnO_2$	1.5	3
$K_{0.4}Fe_{0.1}Mn_{0.8}Ti_{0.1}O_2$	0.5	4
$K_{0.8}CrO_2$	1.08	5
$K_{0.6}Cr_{0.6}Ti_{0.4}O_2$	0.27	This work

Supporting Table S3. Electrode performance of some reported positive electrode materials for K-ion batteries.

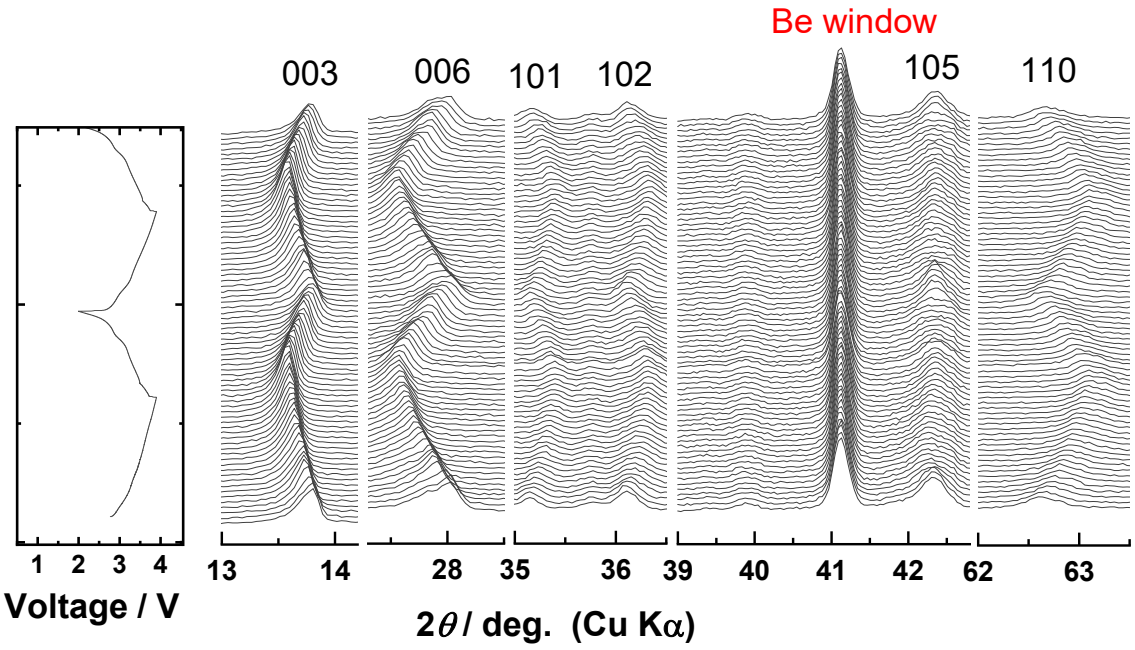
Material	Specific Capacity (mA h g^{-1})	Average Voltage (V)	Cycling Stability (Capacity retention)	Ref.
$K_{0.3}MnO_2$	65 (27.9 mA g^{-1})	2.6	57% (685 cycles)	6
$K_{0.5}MnO_2$	100 (5 mA g^{-1})	2.6	70% (50 cycles)	7
$K_{0.41}CoO_2$	60 (11.8 mA g^{-1})	3.1	95% (30 cycles)	8
$K_{0.6}CoO_2$	80 (2 mA g^{-1})	2.7	60% (120 cycles)	9
$K_{0.69}CrO_2$	85 (100 mA g^{-1})	2.6	65% (1000 cycles)	10
$KCrO_2$	90 (5 mA g^{-1})	2.73	65% (100 cycles)	11
$K_{0.5}Mn_{0.8}Co_{0.1}Ni_{0.1}O_2$	94.5 (20 mA g^{-1})	2.5	63% (300 cycles)	12
$K_{0.48}Mn_{0.4}Co_{0.6}O_2$	64 (C/20)	3	81% (180 cycles)	13
$K_{0.6}Cr_{0.6}Ti_{0.4}O_2$	43 (5 mA g^{-1})	3.14	98% (500 cycles)	This work



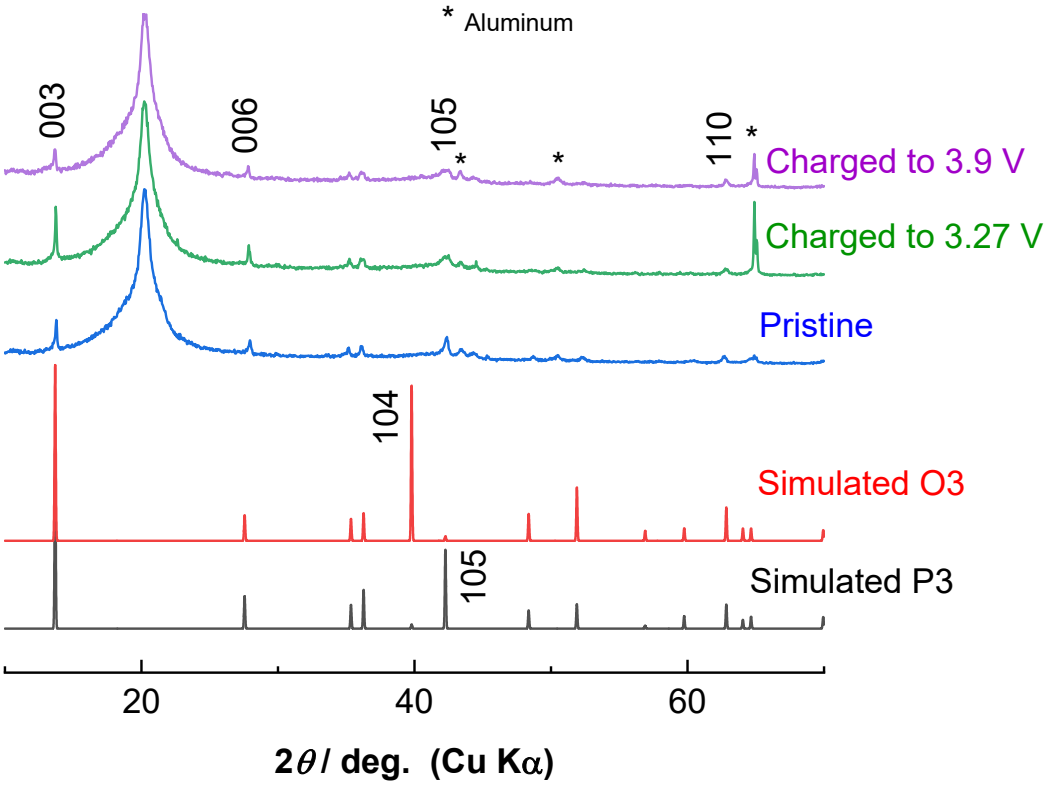
Supporting Figure S1. (a) An XRD pattern of $K_{0.5}Cr_{0.5}Ti_{0.5}O_2$ with schematic illustration of the P3-type layered structure, (b) a SEM image of $K_{0.5}Cr_{0.5}Ti_{0.5}O_2$.



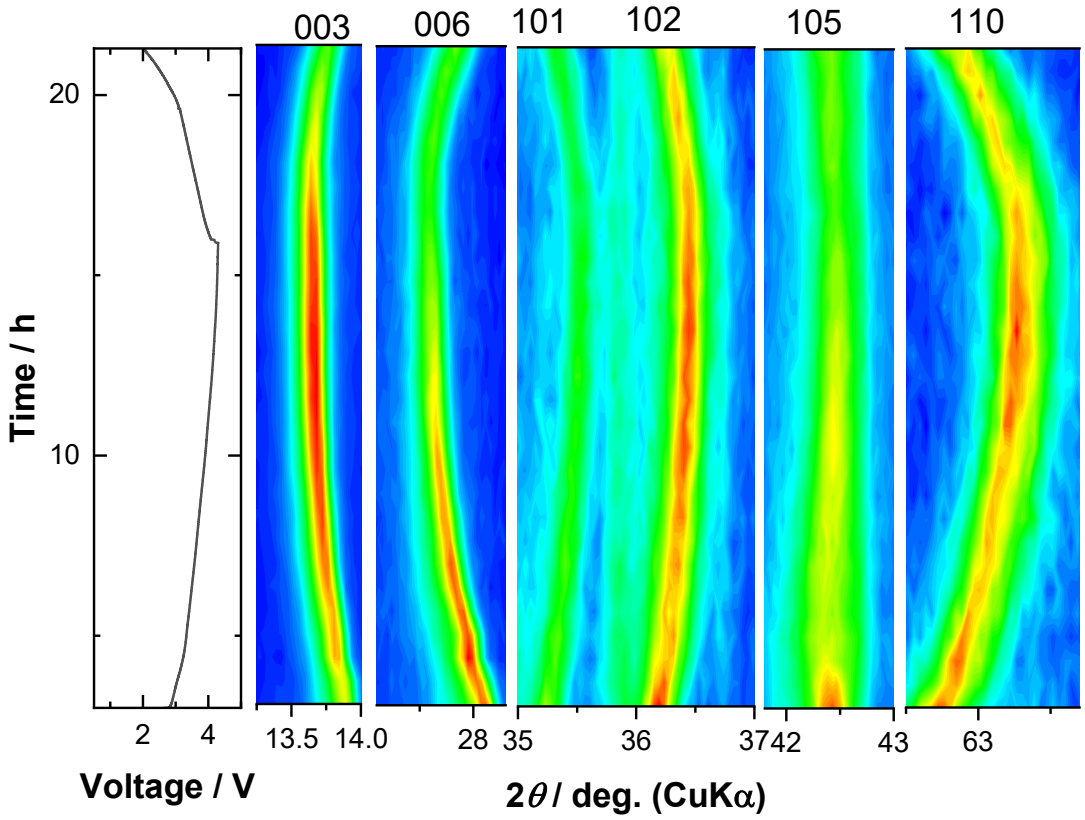
Supporting Figure S2. Charge/discharge profiles of $K_{0.5}Cr_{0.5}Ti_{0.5}O_2$ in the potential range of 2.0 – 4.3 V at a current rate of 5 mA g^{-1}.



Supporting Figure S3. *In-situ* XRD patterns of $K_{0.6-y}Cr_{0.6}Ti_{0.4}O_2$ during charge/discharge.



Supporting Figure S4. *Ex-situ* XRD patterns of $K_{0.6-y}Cr_{0.6}Ti_{0.4}O_2$ at pristine, charged to 3.27 V, and charged to 3.9 V and their comparison with simulated XRD patterns of the O3- and P3-type layered structures. Note that a large and broad peak at 20 degrees originates from Kapton film.



Supporting Figure S5. Contour plots of *in-situ* XRD data of $K_{0.6-y}Cr_{0.6}Ti_{0.4}O_2$ during first cycle in the voltage range of 2.0 – 4.3 V at a rate of 6 mA g^{-1}.

Supporting References

1. K. Lei, Z. Zhu, Z. Yin, P. Yan, F. Li and J. Chen, *Chem*, 2019, **5**, 3220-3231.
2. J. H. Jo, J. U. Choi, Y. J. Park, Y. H. Jung, D. Ahn, T.-Y. Jeon, H. Kim, J. Kim and S.-T. Myung, *Advanced Energy Materials*, 2020, **10**, 1903605.
3. Q. Zhang, C. Didier, W. K. Pang, Y. Liu, Z. Wang, S. Li, V. K. Peterson, J. Mao and Z. Guo, *Advanced Energy Materials*, 2019, **9**, 1900568.
4. X. Zhang, D. Yu, Z. Wei, N. Chen, G. Chen, Z. X. Shen and F. Du, *ACS Applied Materials & Interfaces*, 2021, **13**, 18897-18904.
5. N. Naveen, S. C. Han, S. P. Singh, D. Ahn, K.-S. Sohn and M. Pyo, *Journal of Power Sources*, 2019, **430**, 137-144.
6. C. Vaalma, G. A. Giffin, D. Buchholz and S. Passerini, *Journal of The Electrochemical Society*, 2016, **163**, A1295.
7. H. Kim, D.-H. Seo, J. C. Kim, S.-H. Bo, L. Liu, T. Shi and G. Ceder, *Advanced Materials*, 2017, **29**, 1702480.
8. Y. Hironaka, K. Kubota and S. Komaba, *Chemical Communications*, 2017, **53**, 3693-3696.

9. H. Kim, J. C. Kim, S.-H. Bo, T. Shi, D.-H. Kwon and G. Ceder, *Advanced Energy Materials*, 2017, **7**, 1700098.
10. J.-Y. Hwang, J. Kim, T.-Y. Yu, S.-T. Myung and Y.-K. Sun, *Energy & Environmental Science*, 2018, **11**, 2821-2827.
11. H. Kim, D.-H. Seo, A. Urban, J. Lee, D.-H. Kwon, S.-H. Bo, T. Shi, J. K. Papp, B. D. McCloskey and G. Ceder, *Chemistry of Materials*, 2018, **30**, 6532-6539.
12. L. Duan, Y. Xu, Z. Zhang, J. Xu, J. Liao, J. Xu, Y. Sun, Y. He and X. Zhou, *Journal of Materials Chemistry A*, 2021, **9**, 22820-22826.
13. K. Sada and P. Barpanda, *Chemical Communications*, 2020, **56**, 2272-2275.