Supporting Information for

$ATiOPO_4$ (A=NH_4, K, Na): Novel 1.5 V Anode Material as Room-temperature Sodium Battery

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Supplementary Tables

Supporting Tables 1 The lattice parameters caculated from Rietveld refinement for the as-prepared NTP (a), KTP (b) and NaTP (c) samples.

(a)

	a	b	c	α=β=γ	Rwp	*Rp*	*gof*
NTP	12.9210(1)	6.4991(3)	10.5870(2)	90°	10.582%	7.819%	1.642
		X	Y	Z			
	NH_4(1)	0.3821(5)	0.7962(0)	0.3080(1)			
	NH_4(2)	0.1170(5)	0.6995(2)	0.0761(3)			
	O1	0.4823(3)	0.4829(1)	0.1477(2)			
	O2	0.5166(1)	0.4593(2)	0.3716(0)			
	O3	0.4138(9)	0.1673(2)	0.3260(1)			
	O4	0.5955(2)	0.1948(3)	0.2518(4)			
	O5	0.1191(5)	0.2908(2)	0.5286(5)			
	O6	0.1201(6)	0.6590(1)	0.4588(3)			
	O7	0.2506(2)	0.5457(6)	0.6338(5)			
	O8	0.2529(2)	0.4590(2)	0.3967(2)			
	OT1	0.2613(0)	0.4264(1)	0.1444(0)			
	OT2	0.2778(1)	0.5315(2)	0.8672(4)			
	P1	0.4983(6)	0.3333(1)	0.2344(0)			
	P2	0.1850(0)	0.5053(1)	0.5097(0)			
	Ti1	0.3724(1)	0.4949(2)	-0.0087(1)			
	Ti2	0.2508(4)	0.2645(0)	0.2473(0)			

(b)

	a	b	c	α=β=γ	Rwp	*Rp*	*gof*
KTP	12.8201(2)	6.4111(1)	10.5804(2)	90°	9.584%	7.210%	1.876
		X	Y	Z			
	K(1)	0.3746(4)	0.7865(0)	0.3022(6)			
	K(2)	0.1054(3)	0.6989(2)	0.0755(3)			
	O1	0.4834(2)	0.4697(5)	0.1466(4)			
	O2	0.5188(1)	0.4755(7)	0.3942(0)			
	O3	0.4045(1)	0.2147(1)	0.2735(1)			
	O4	0.5820(2)	0.2175(3)	0.2663(4)			
	O5	0.1194(3)	0.3255(5)	0.5787(1)			
	O6	0.0964(0)	0.7009(3)	0.4679(5)			
	O7	0.2526(2)	0.5656(1)	0.6284(5)			
	O8	0.2530(0)	0.4600(7)	0.3956(0)			
	OT1	0.2649(5)	0.4563(7)	0.1206(9)			
	OT2	0.2778(9)	0.5417(6)	0.8898(0)			
	P1	0.4947(6)	0.3288(4)	0.2595(0)			
	P2	0.1863(8)	0.4986(2)	0.5050(6)			
	Ti1	0.3755(0)	0.5077(4)	0.0014(2)			
	Ti2	0.2451(4)	0.2674(5)	0.2412(4)			

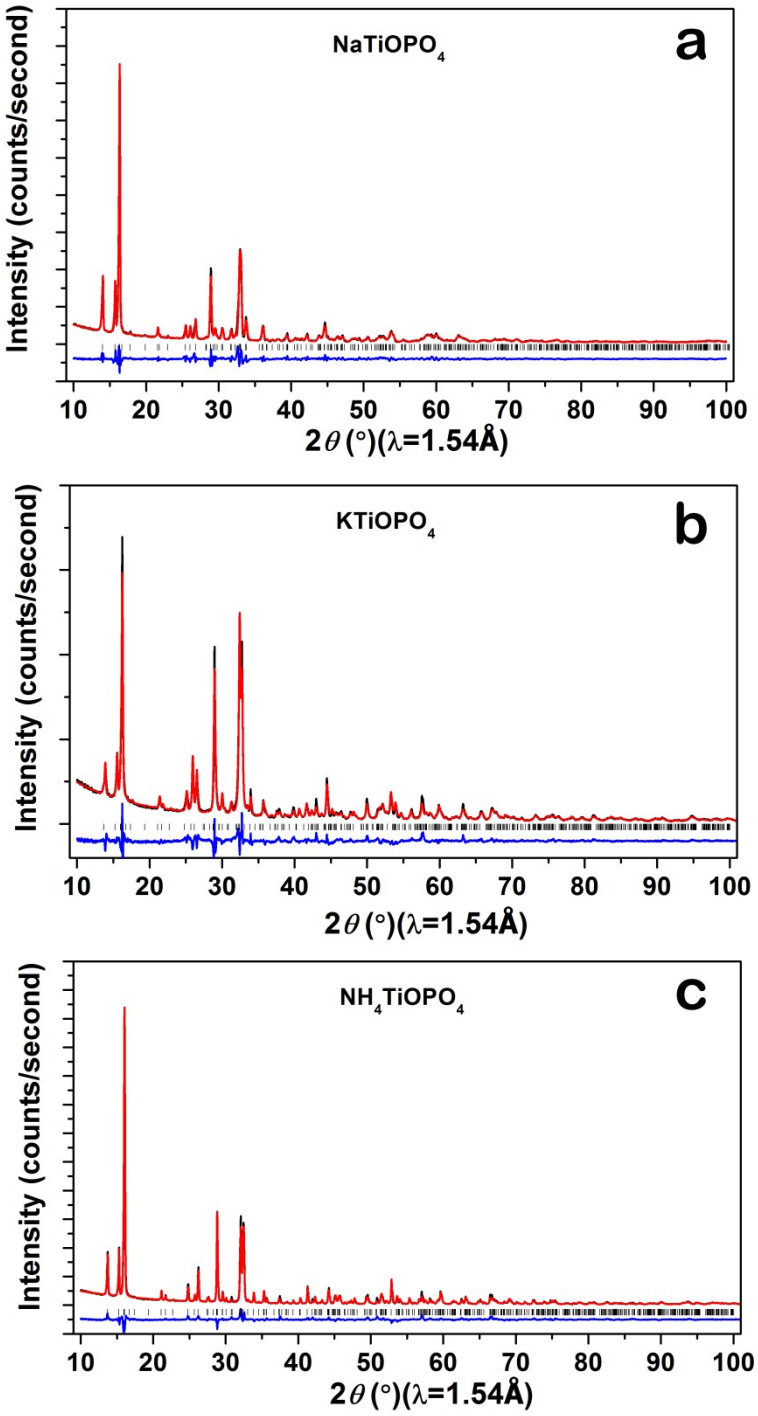
(c)

	a	b	c	α=β=γ	Rwp	*Rp*	*gof*
NaTP	12.6248(3)	6.2912(1)	10.6211(1)	90°	10.531%	7.544%	1.693
		X	Y	Z			
	Na(1)	0.3522(2)	0.8019(0)	0.2819(1)			
	Na(2)	0.0956(0)	0.7273(2)	0.0657(3)			
	O1	0.4807(2)	0.5061(1)	0.1494(2)			
	O2	0.5112(0)	0.4390(7)	0.3917(0)			
	O3	0.3746(1)	0.2199(0)	0.2846(1)			
	O4	0.5779(3)	0.1890(3)	0.2461(2)			
	O5	0.1482(3)	0.3543(1)	0.5805(2)			
	O6	0.1092(0)	0.7061(3)	0.4990(3)			
	O7	0.2611(3)	0.5698(1)	0.6230(1)			
	O8	0.2343(1)	0.4778(4)	0.3732(0)			
	OT1	0.2618(5)	0.4719(0)	0.1308(3)			
	OT2	0.2879(2)	0.5405(3)	0.8828(0)			
	P1	0.4819(0)	0.3382(4)	0.2698(0)			
	P2	0.1935(5)	0.5057(1)	0.5008(6)			
	Ti1	0.3693(0)	0.5274(0)	0.0012(2)			
	Ti2	0.2374(1)	0.2863(4)	0.2364(2)			

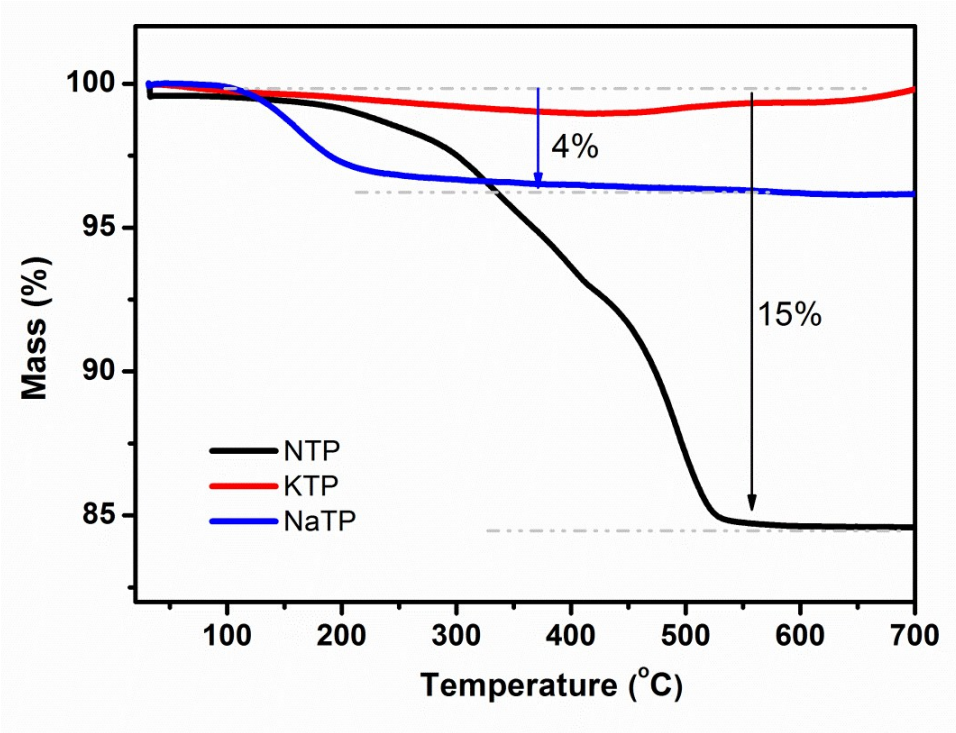
Supporting Tables 2 EDS results for NTP, KTP and NaTP samples.

	K	Na	Ti	P	O
NH_4TiOPO_4	-	-	11.3	10.86	69
$KTiOPO_4$	9	-	9.38	10.18	77
$NaTiOPO_4$	-	10.02	9.84	11	76

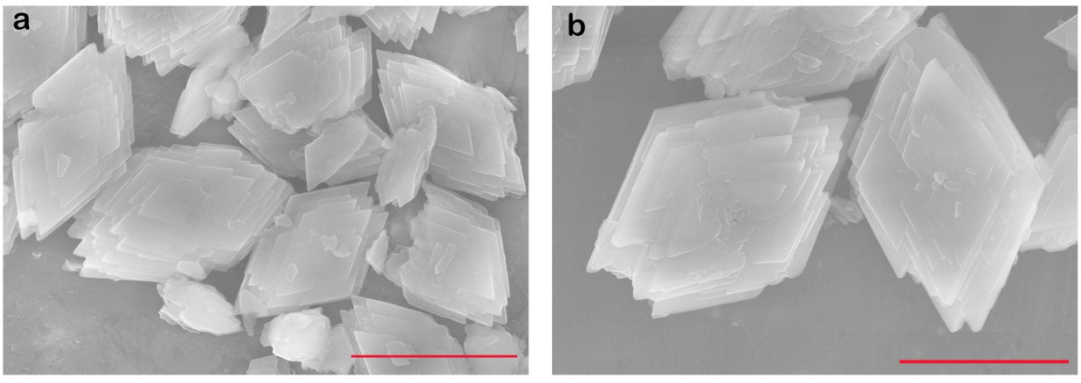
Supplementary Figures



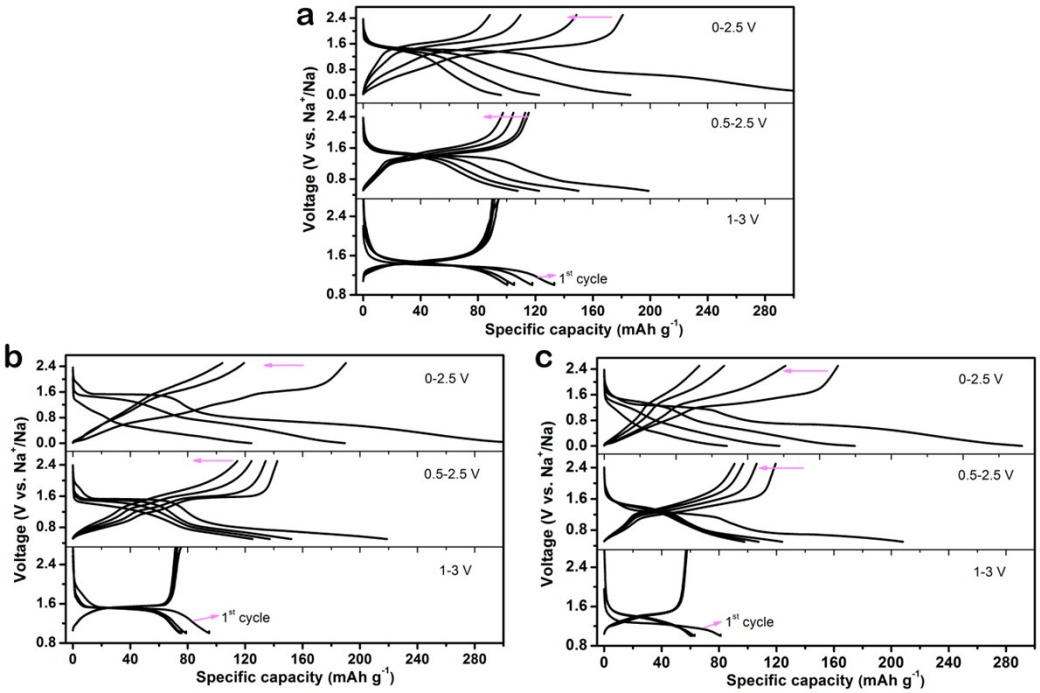
Supporting Fig. S1 XRD patterns from Rietveld refinement for NTP (c), KTP (b) and NaTP (a) samples. All XRD patterns were refined using the Rietveld method, as implemented in the program TOPAS.



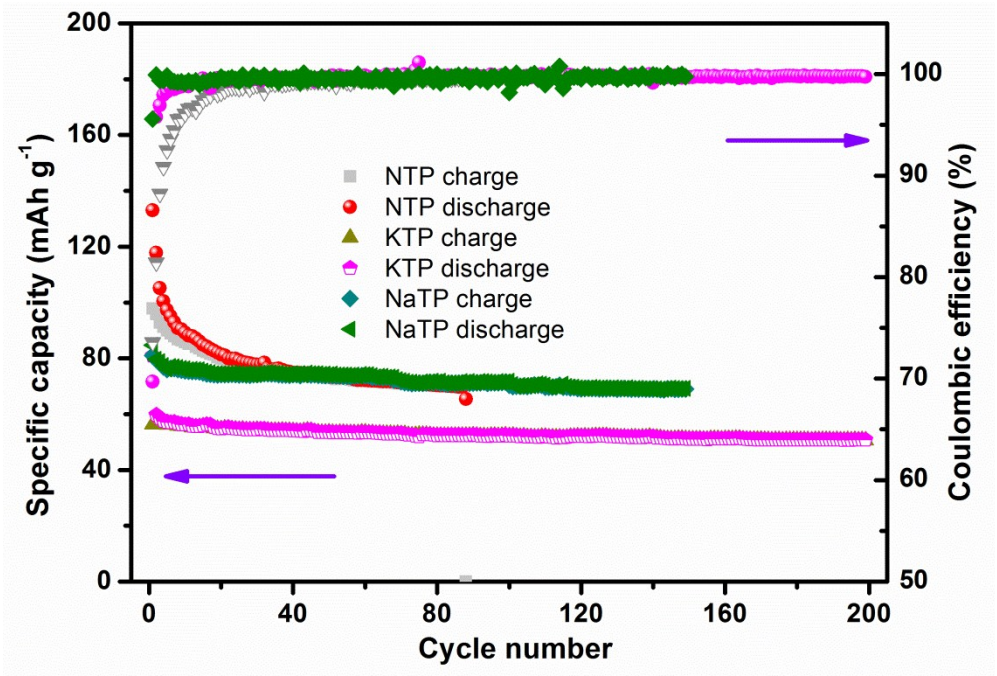
Supporting Fig. S2 TG profiles for NTP, KTP and NaTP samples. The heating temperature range is 25°C-800°C in Ar/O_2 atmosphere.



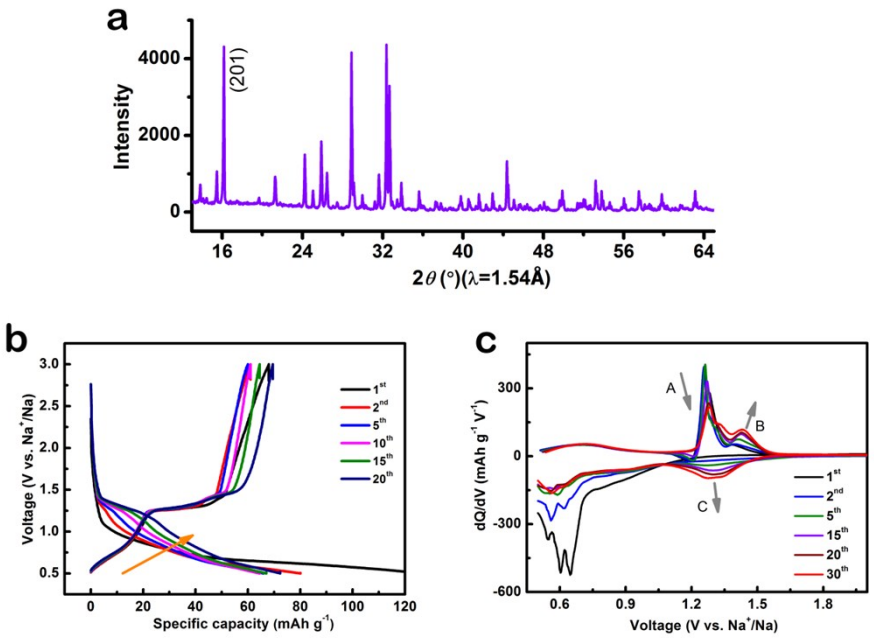
Supporting Fig. S3 Typical morphologies for KTP (a) and NaTP (b) samples. The scale bar is 2 μm.



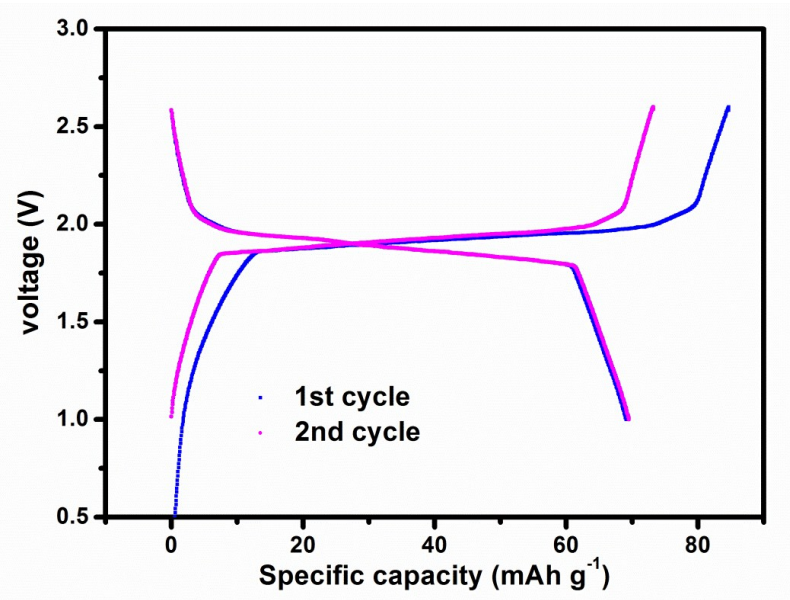
Supporting Fig. S4 Discharge and charge curves for NTP (a), NaTP (b) and KTP (c) electrode in different voltage ranges.



Supporting Fig. S5 Long-term cycling performance for NTP, KTP and NaTP electrode in the voltage rang of 1.0-3.0 V.



Supporting Fig. S6 XRD pattern of SS-KTP sample (a), discharge and charge (b) and corresponding dQ/dV curves for SS-KTP electrode.



Supporting Fig. S7 The first and second charge/discharge profiles of full cell with NaTP as anode and $Na_3V_2(PO_4)$ as cathode at a current rate of C/10. (The specific capacity is calculated based on anode mass)