Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

SUPPORTING INFORMATION

Reversible facile monovalent K^+ and Rb^+ ions de/insertion in a $KTiOPO_4$-type $RbVPO_4F$ cathode material

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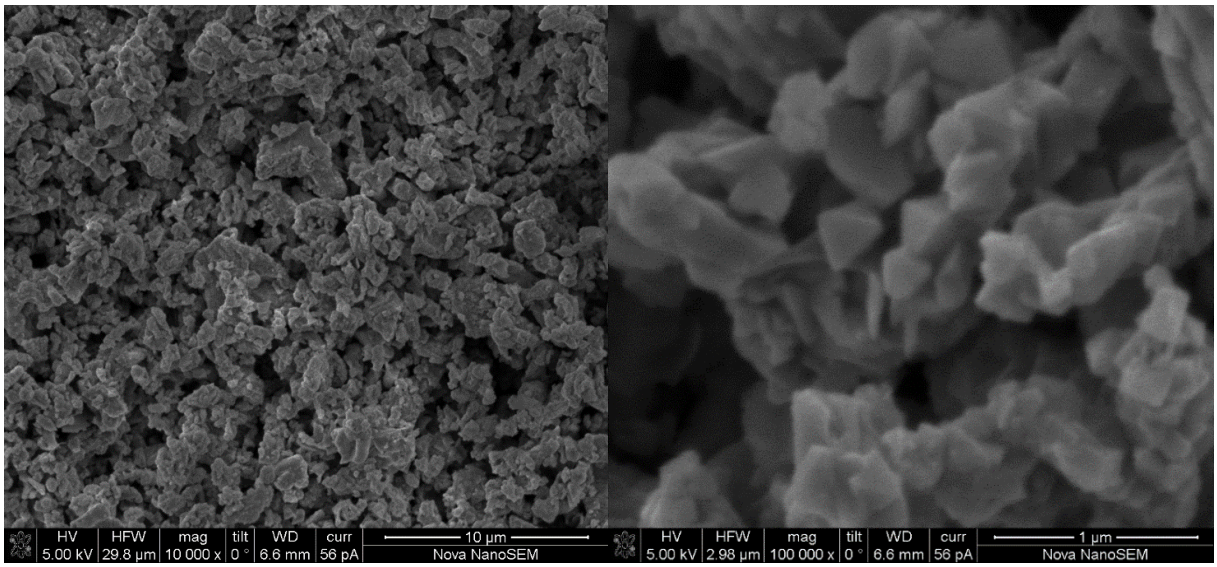

Figure S1. SEM micrographs of $RbVPO_4F$ at 10Kx and 100Kx magnifications.

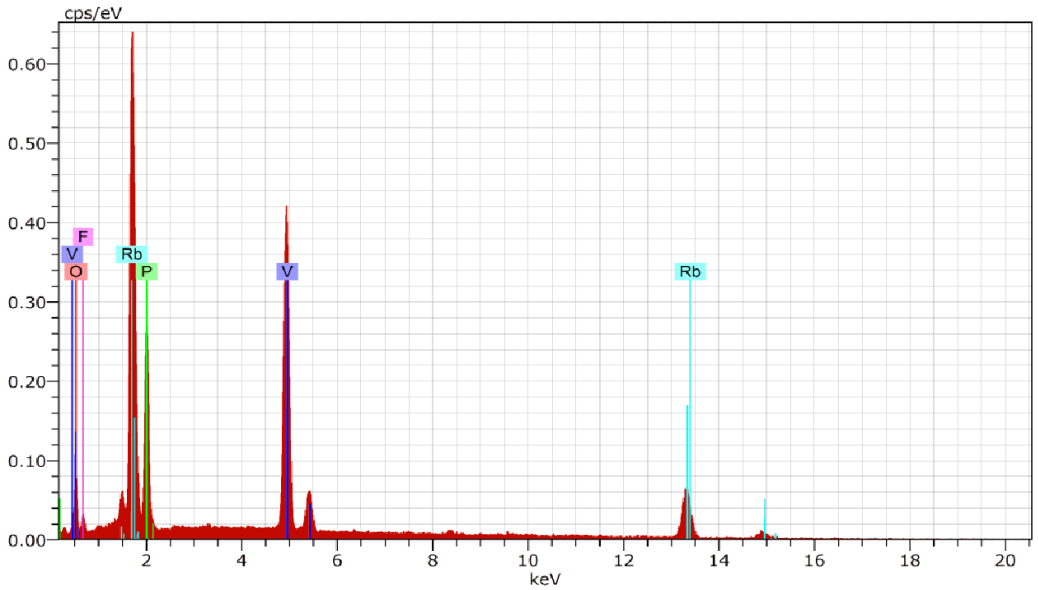

Figure S2. SEM-EDX spectrum for $RbVPO_4F$.

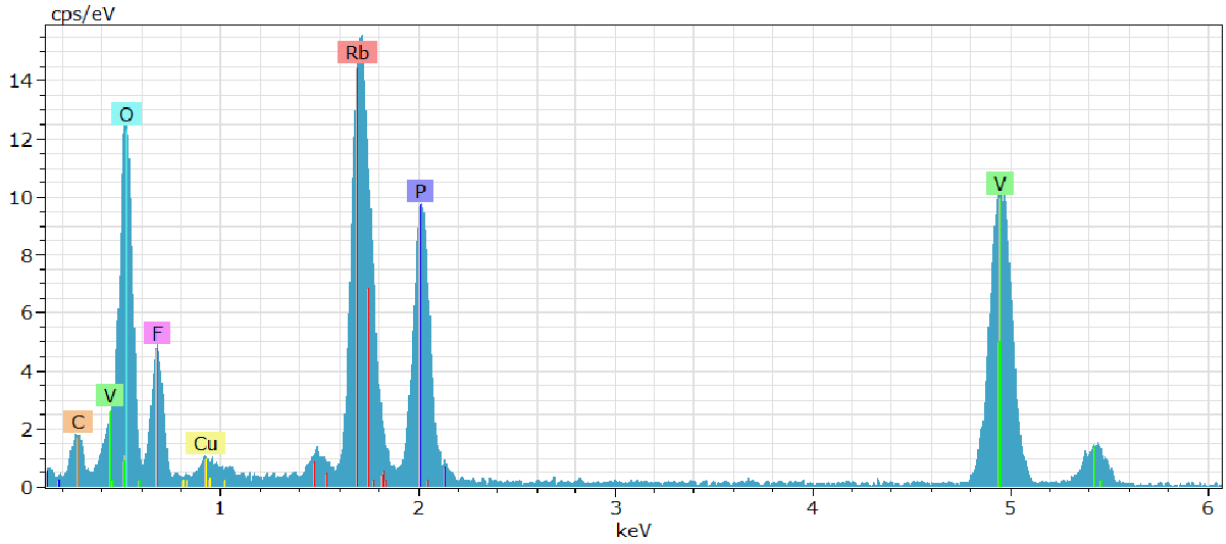

Figure S3. TEM-EDX spectrum for $RbVPO_4F$.

Table S1. Fractional atomic coordinates and atomic displacement parameters for $RbVPO_4F$.

Atom	Wyckoff	*x/a*	*y/b*	*z/c*	*V*, Å^3	Occupation
P1	4d	0.4977(7)	0.3246(10)	0.2440(12)	0.034(2)	1
P2	4d	0.1787(5)	0.4845(16)	0.4986(10)	0.017(2)	1
V1	4d	0.3842(3)	0.4971(10)	0	0.0210(15)	1
V2	4d	0.2506(5)	0.2591(10)	0.2525(8)	0.0243(15)	1
F1	4d	0.2735(15)	0.465(2)	0.1199(11)	0.019(3)	1
F2	4d	0.2264(13)	0.018(3)	0.3629(12)	0.019(3)	1
O1	4d	0.0167(16)	0.027(3)	0.3515(14)	0.0078(14)	1
O2	4d	0.4807(16)	0.466(3)	0.1304(16)	0.0078(14)	1
O3	4d	0.0955(13)	0.299(2)	0.2199(18)	0.0078(14)	1
O4	4d	0.4038(14)	0.198(3)	0.2742(15)	0.0078(14)	1
O5	4d	0.1145(13)	0.681(3)	0.4655(16)	0.0078(14)	1
O6	4d	0.3939(13)	0.805(3)	0.0384(16)	0.0078(14)	1
O7	4d	0.2556(14)	0.431(2)	0.3991(15)	0.0078(14)	1
O8	4d	0.2590(13)	0.006(3)	0.1186(14)	0.0078(14)	1
Rb1	4d	0.1220(9)	0.7408(14)	0.1888(12)	0.0338(16)	0.5
Rb1'	4d	0.1045(10)	0.6893(17)	0.1685(10)	0.0338(16)	0.5
Rb2	4d	0.3897(9)	0.7973(18)	0.4003(7)	0.0180(15)	0.5
Rb2'	4d	0.3972(7)	0.8088(14)	0.4496(9)	0.0180(15)	0.5

Table S2. Selected interatomic distances for $RbVPO_4F$.

Bond	Distance, Å	Bond	Distance, Å
V1–O1	2.040(19)	V2–O3	2.063(18)
V1–O2	1.87(2)	V2–O4	2.04(2)
V1–O5	2.089(18)	V2–O7	1.914(17)
V1–O6	2.048(19)	V2–O8	2.175(19)
V1–F1	1.929(17)	V2–F1	1.963(16)
V1–F2	2.045(16)	V2–F2	1.981(17)
P2–O5	1.568(19)	P1–O1	1.51(2)
P2–O6	1.56(2)	P1–O2	1.53(2)
P2–O7	1.492(19)	P1–O3	1.527(18)
P2–O8	1.512(19)	P1–O4	1.51(2)
Rb1–O1	2.88(2)	Rb2–O1	2.73(2)
Rb1–O2	2.72(2)	Rb2–O2	3.42(2)
Rb1–O3	2.914(16)	Rb2–O3	3.38(2)
Rb1–O5	2.95(2)	Rb2–O4	2.93(2)
Rb1–O6	2.38(2)	Rb2–O5	3.01(2)
Rb1–O7	3.466(19)	Rb2–O7	2.952(19)
Rb1–O8	2.59(2)	Rb2–O8	3.557(19)
Rb1–F1	2.76(2)	Rb2–F1	3.328(18)
Rb1–F2	2.913(19)	Rb2–F2	2.59(2)
Rb1–Rb1’	0.459(16)	Rb2–Rb2’	0.535(12)
Rb1'–O1	3.14(2)	Rb2’–O1	2.88(2)
Rb1'–O2	2.79(2)	Rb2’–O2	3.06(2)
Rb1'–O3	2.600(18)	Rb2’–O3	2.86(2)
Rb1'–O5	3.14(2)	Rb2’–O4	3.141(19)
Rb1'–O6	3.06(2)	Rb2’–O5	2.830(19)
Rb1'–O7	3.55(2)	Rb2’–O7	3.116(17)
Rb1'–O8	2.93(2)	Rb2’–O8	3.346(19)
Rb1'–F1	2.69(2)	Rb2’–F1	3.032(19)
Rb1’–F2	3.364(19)	Rb2’–F2	2.761(19)
Rb1’–Rb2’	3.389(14)		

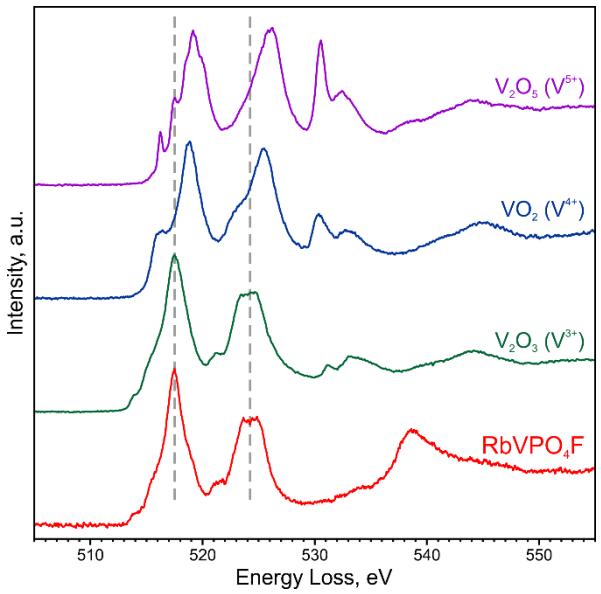

Figure S4. EELS spectrum in the vicinity of the VL2,3 edge for $RbVPO_4F$ compared to known spectra of V in octahedral coordination.

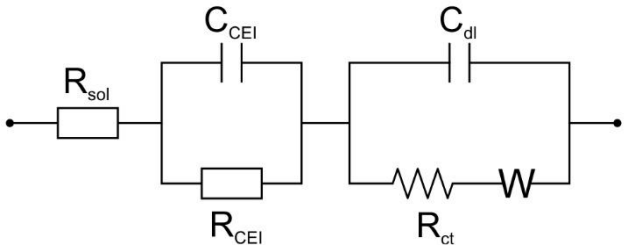

Figure S5. Equivalent circuit for the intercalation reaction. R_{sol} – uncompensated solution resistance; C_{CEI} – CEI capacitance; R_{CEI} – CEI resistance; C_{dl} – double layer capacitance; R_{ct} – charge transfer resistance; W – Warburg impedance.