energies

Supplementary Materials:

Synthesis, Structure and Sodium Mobility of Sodium Vanadium Nitridophosphate: A Zero-Strain and Safe High Voltage Cathode Material for Sodium-ion Batteries

Huang Zhang, Daniel Buchholz and Stefano Passerini

Table S1. Crystallographic data of $Na_3V(PO_3)_3N$.

	Value
Chemical formula	$Na_3V(PO_3)_3N$
Crystal system, space group	Cubic, $P2_13$
R-bragg	9.7%
Cell mass	1483.3
Cell volume ($Å^3$)	841.3 (9)
Crystal density (g cm^{-3})	2.9307 (3)
Temperature	~298 K (ambient)
Lattice parameters	-
a (Å)	9.440 (1)
R_{wp}	8.7%
R_p	6.7%
GOF	1.41
Radiation type	Cu K_α, λ = 1.541(8) Å

Table S2. Atomic parameters for $Na_3V(PO_3)_3N$.

Site	**x***	**y***	**z***		**Occ***	**B_{eq}***
Na1	−0.26140	0.73860	0.73860	Na^+	1	0.0255
Na2	0.14230	0.64230	0.85770	Na^+	1	0.0181
Na3	−0.05180	0.94820	0.94820	Na^+	1	0.029
V1	0.33070	0.83070	0.66930	V^{3+}	1	0.0109
P1	0.00415	0.83568	0.58270	P^{5+}	1	0.0092
N1	0.05150	0.94850	0.44850	N^{3-}	1	0.0087
O1	−0.09860	0.72930	0.52000	O^{2-}	1	0.0154
O2	0.13720	0.75680	0.62370	O^{2-}	1	0.0124
O3	−0.06150	0.91810	0.70020	O^{2-}	1	0.017

* fixed parameters

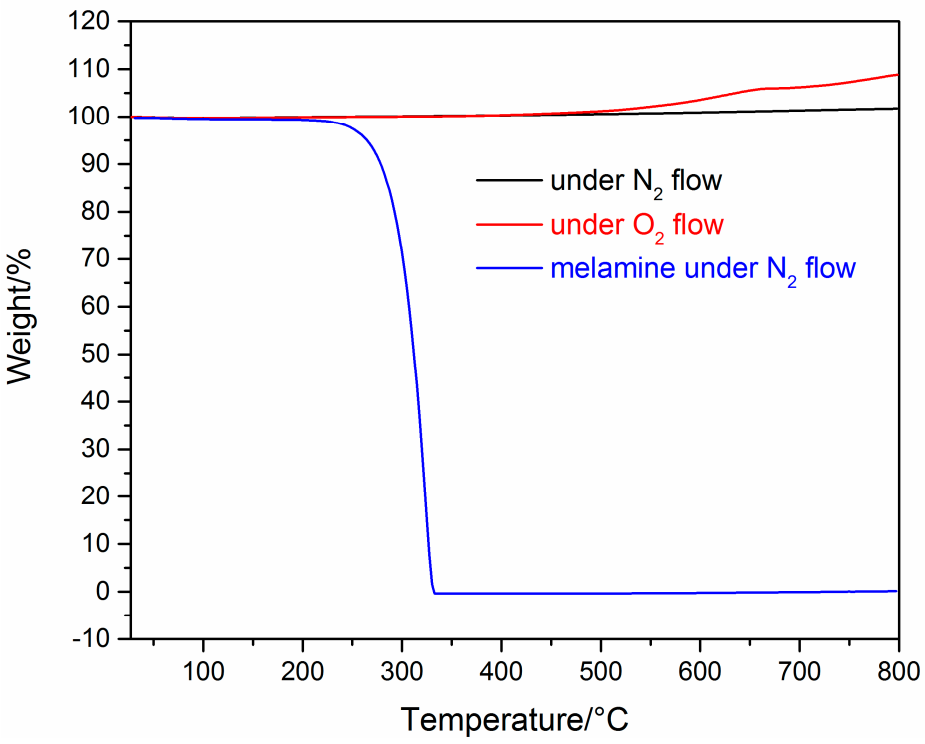

Figure S1. TG curves of $Na_3V(PO_3)_3N$ under N_2 and O_2 flows and melamine under N_2 flow of 20 ml min^{-1} within the temperature range of 30–800 °C at 5 °C min^{-1} heating rate.

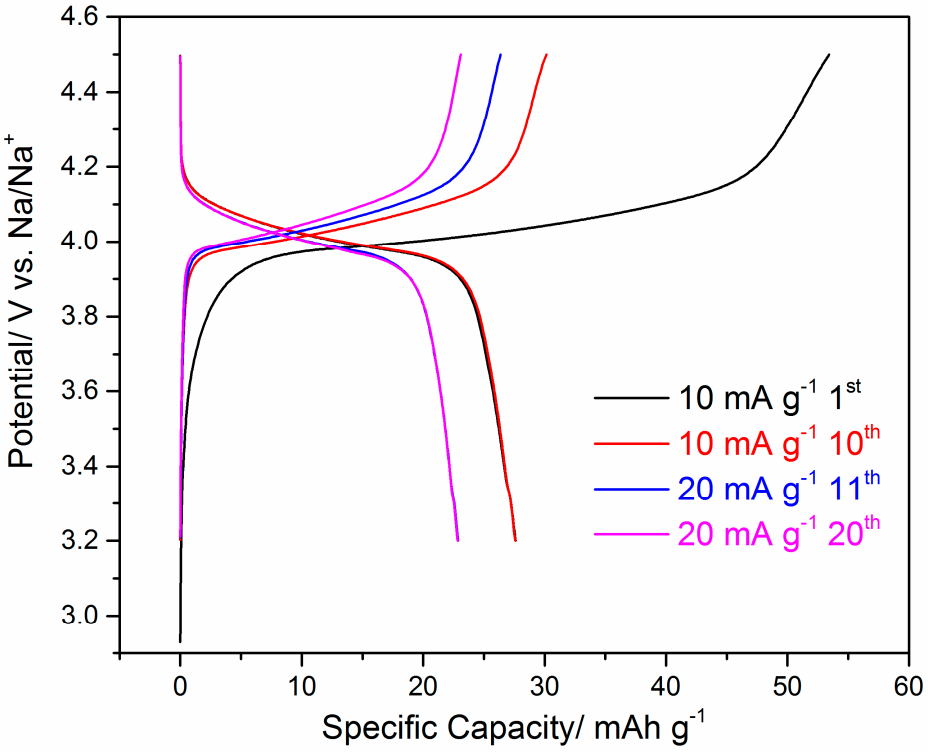

Figure S2. Galvanostatic charge-discharge profiles of $Na_3V(PO_3)_3N$ at current density of 10 mA g^{-1} for the 1st and 10th cycles and 20 mA g^{-1} for 11th and 20th cycles.

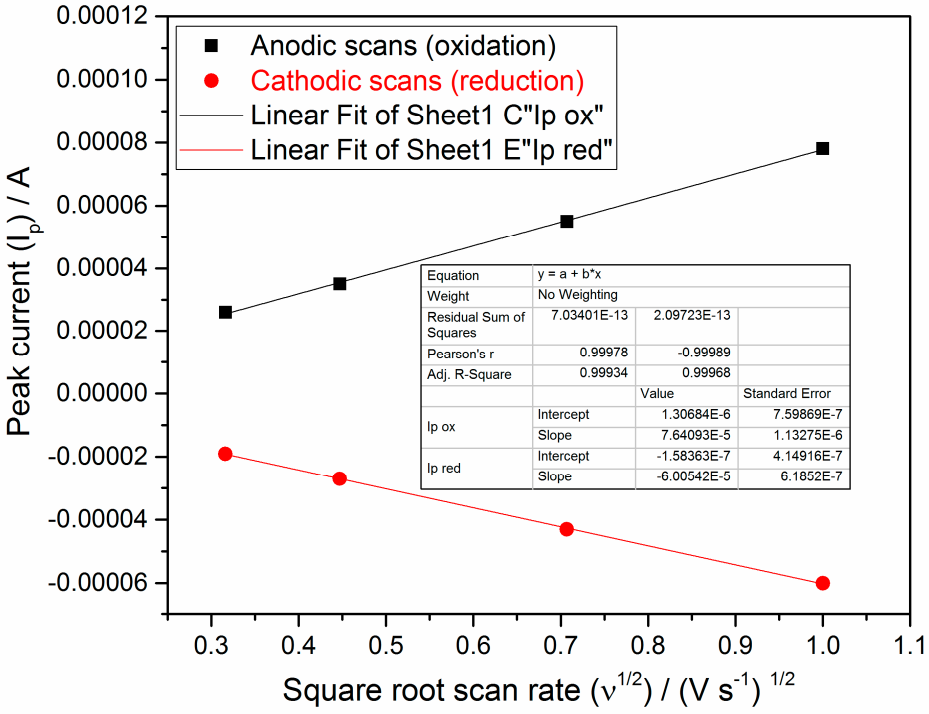

Figure S3. Peak current (I_P, A cm^{-2}) vs. square root of scan rate ($v^{1/2}$, $V^{1/2}$ $s^{-1/2}$) and related linear fit corresponding to the $V^{3+/4+}$ redox processes.

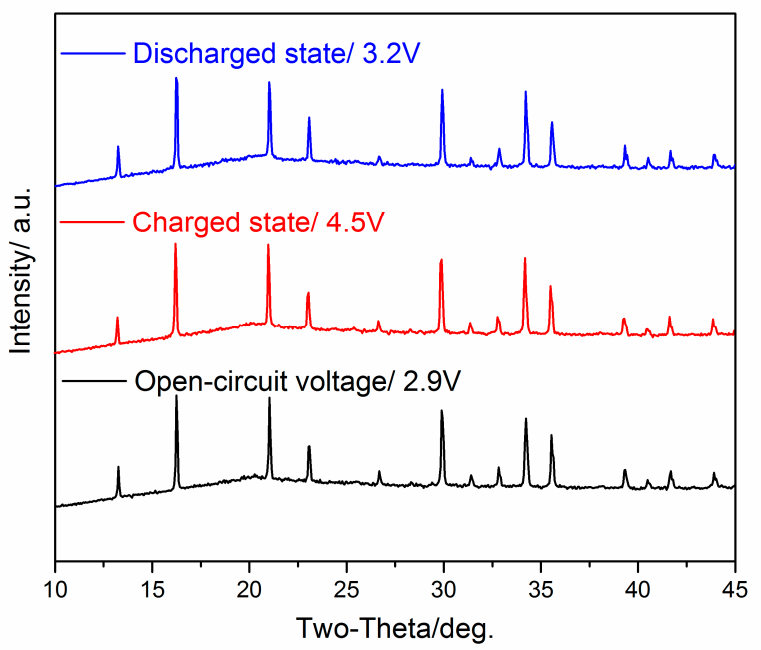

Figure S4. In-situ X-ray diffraction patterns of $Na_3V(PO_3)_3N$ at OCV, after the 1st charge (4.5 V) and 1st discharge state (3.2 V).