Supporting Information

Stable Vacancy-Rich Sodium Vanadate as a Cathode for High-Performance Aqueous Zinc-Ion Batteries

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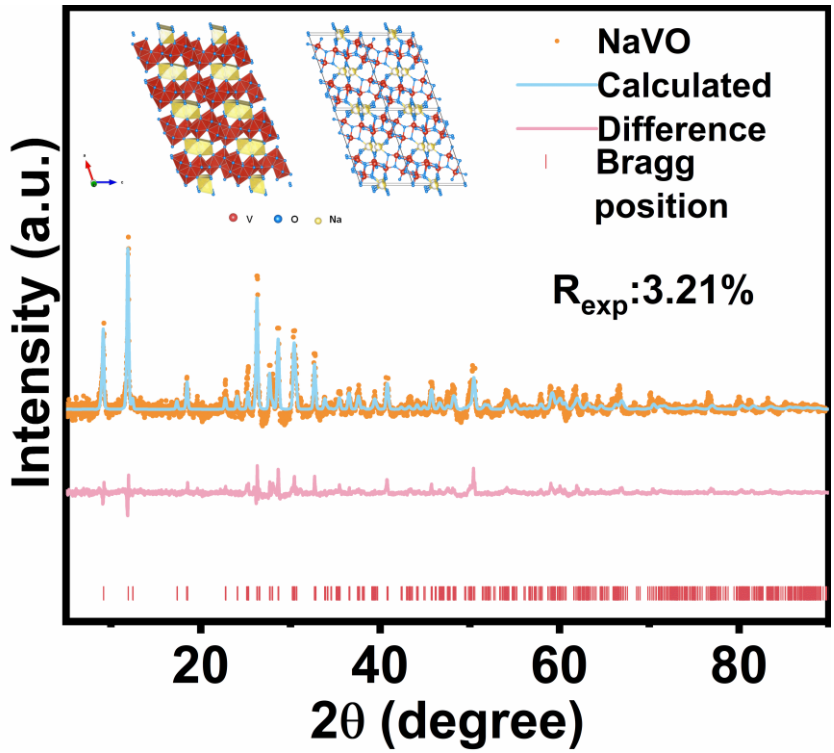


Figure S1. The crystal structure and the Rietveld refinement of NaVO.

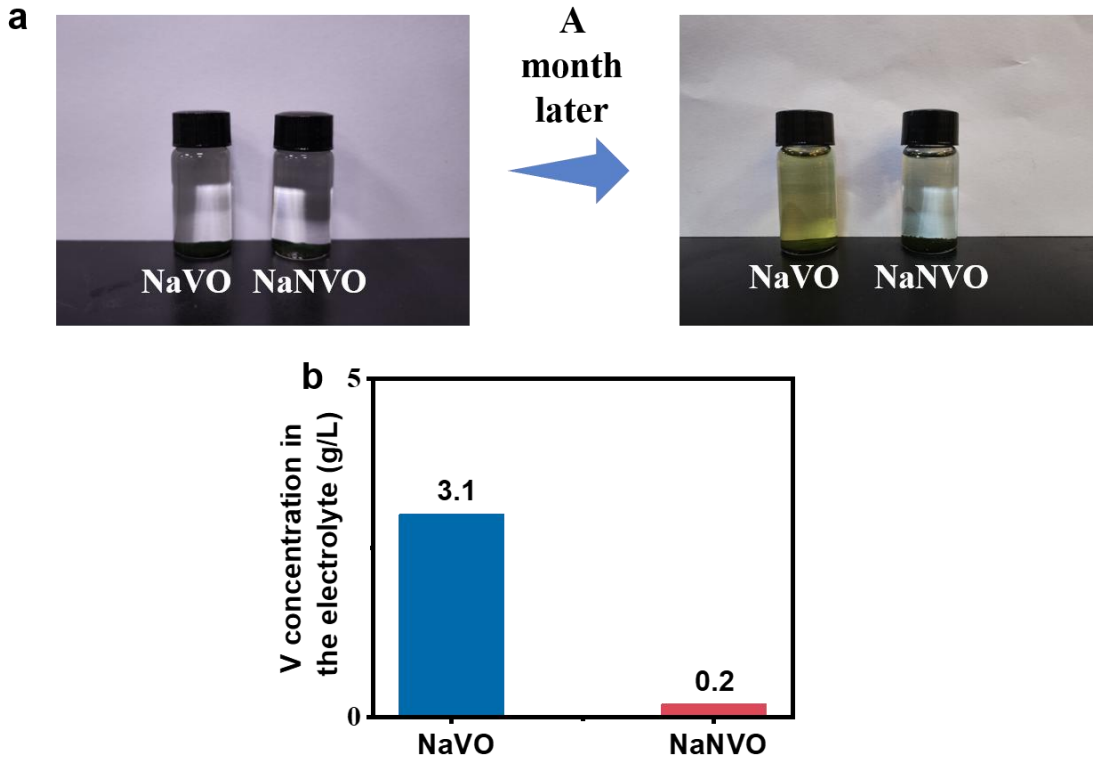


Figure S2. Comparison on the dissolution ability of the electrode materials in the electrolytes (a) The color change implies the stability difference between NaNVO and NVO after immerse in electrolyte over one month. (b) The concentration of vanadium dissolved in the electrolyte confirmed by the Induc-tively coupled plasma-optical emission spectrometry (ICP-OES).

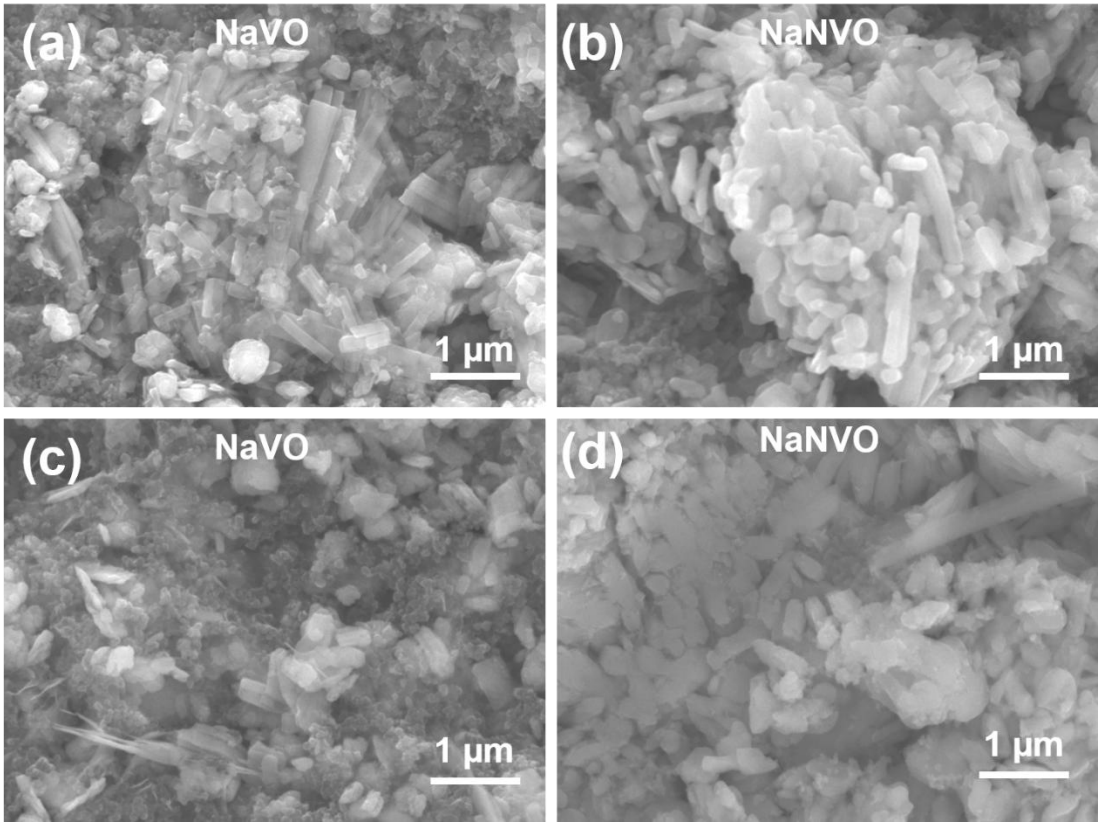


Figure S3. SEM of different cathode materials before cycling: (a) NaVO, (b) NaNVO. SEM of different cathode materials after 50th: (c) NaVO, (d) NaNVO.

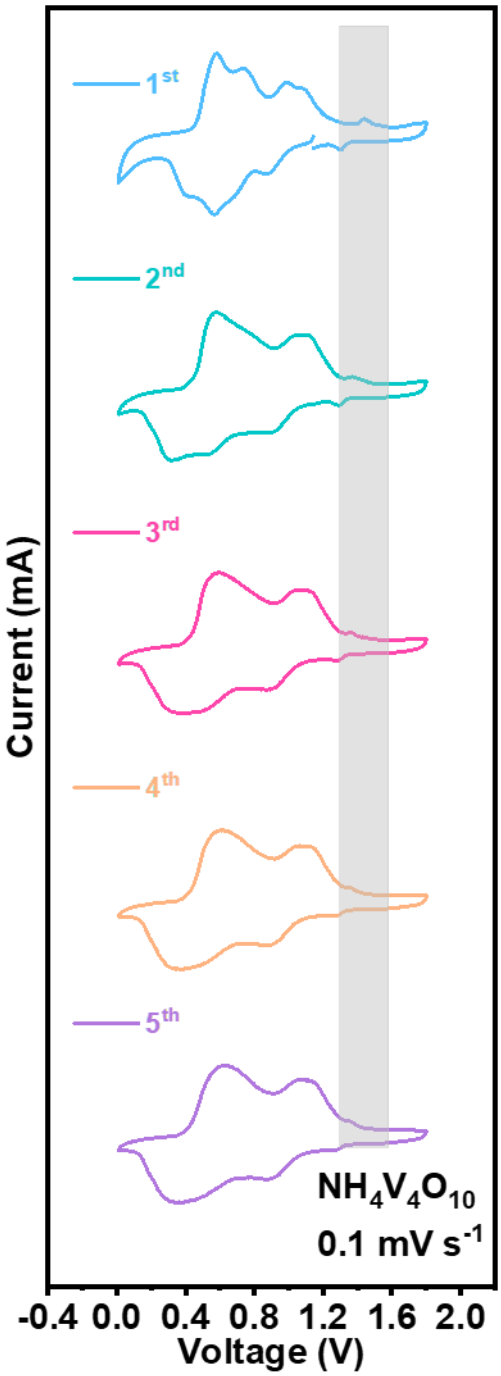


Figure S4. CV curve of $NH_4V_4O_{10}$.

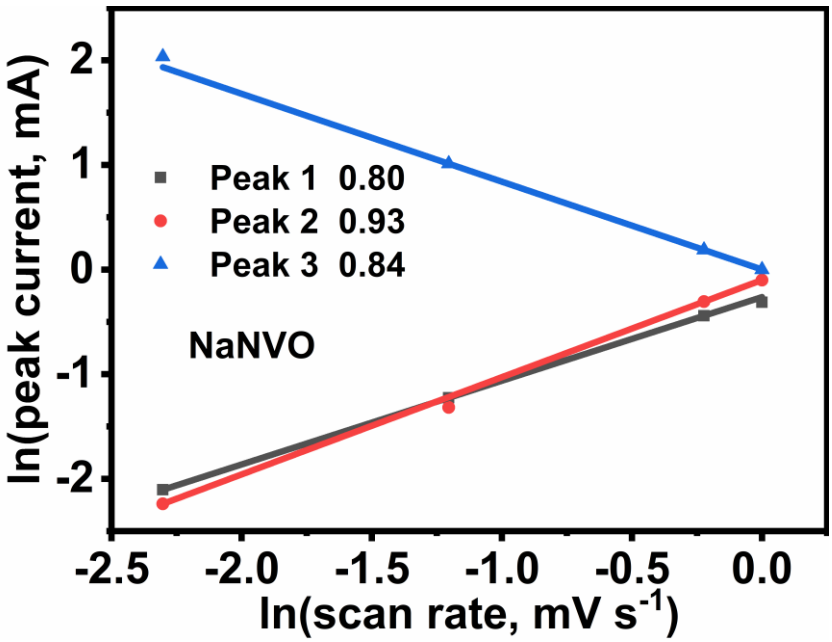


Figure. S5. The relationship between peak currents and sweep rates, and corresponding b values of NaNVO.

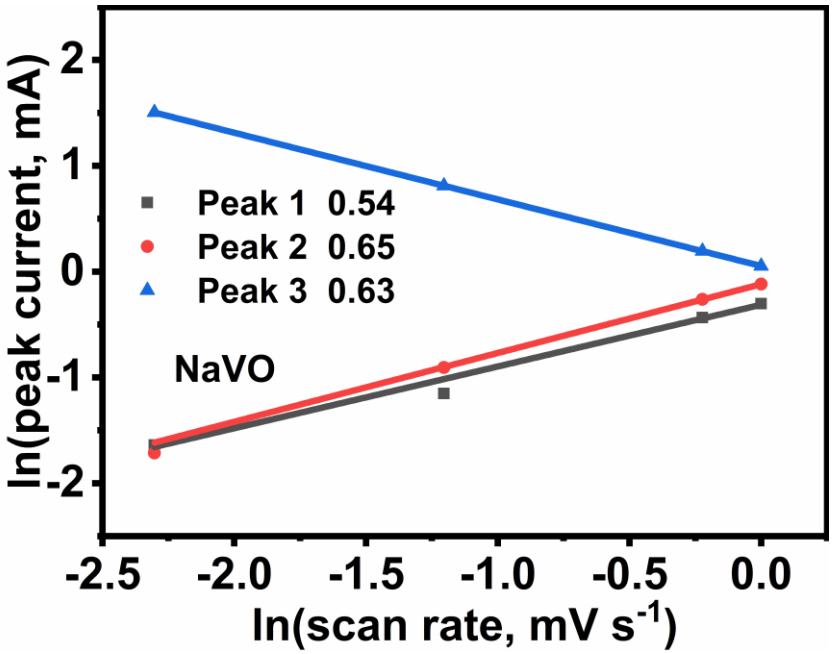


Figure S6. The relationship between peak currents and sweep rates, and corresponding b values of NaVO.

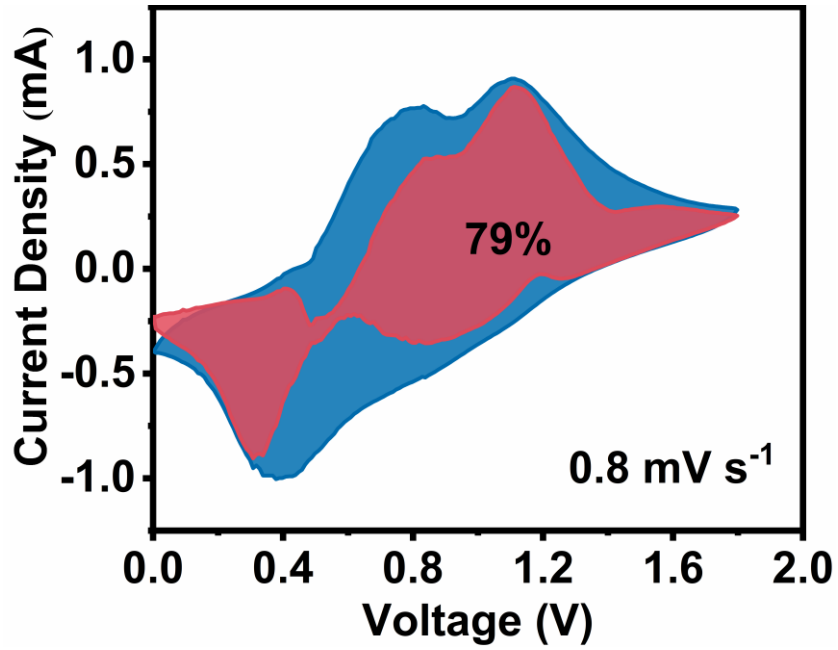


Figure S7. Capacitive contribution of the NaNVO cathode at the sweet rate of 0.8 mV s^{-1}

Table S1. The cellular parameters of NaVO

Atom	Site	x	y	z	g (occupancy)
Na	4i	0.00456	0	0.40374	0.396
V1	4i	0.33698	0	0.10205	0.988
V2	4i	0.11566	0	0.11889	0.989
V3	4i	0.29079	0	0.41401	0.988
O1	2a	0	0	0	0.926
O2	4i	0.81829	0	0.06433	0.932
O3	4i	0.63535	0	0.0819	1.016
O4	4i	0.43762	0	0.2244	1.011
O5	4i	0.26598	0	0.22451	0.881
O6	4i	0.11249	0	0.27983	1.006
O7	4i	0.7595	0	0.42476	0.975
O8	4i	0.40054	0	0.46892	1.014

NaVO space group: C 2/m

a =10.096 Å, = 3.608 Å, = 15.583 Å, = 536.117 Å

Table S2. The cellular parameters of NaNVO

Atom	Site	x	y	z	g (occupancy)
Na	4i	-0.02202	0	0.43078	0.215
NH4	4i	-0.04442	0	0.23456	0.189
V1	4i	0.33412	0	0.10479	1.019
V2	4i	0.11633	0	0.11971	0.982
V3	4i	0.28815	0	0.41837	0.993
O1	2a	0	0	0	0.855
O2	4i	0.8126	0	0.05509	0.884
O3	4i	0.61949	0	0.09235	1.004
O4	4i	0.43704	0	0.2282	1.006
O5	4i	0.25769	0	0.21172	0.886
O6	4i	0.11226	0	0.25678	1.014
O7	4i	0.73442	0	0.4154	0.892
O8	4i	0.4081	0	0.47731	1.022
NaNVO space group: C 2/m					
a =10.089 Å, b = 3.608 Å, c = 15.394 Å, V = 527.989 Å^3					

Table S3. The stoichiometry results for NaVO and NaNVO.

Samples	Measured atomic radio by ICP-OES	
	Na	V
NaVO	0.78	6.05
NaNVO	0.41	5.98

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Table S4. Comparison of the electrochemical properties of some vanadium-based cathode materials.

Cathode material	Electrolyte	Capacit	Energy density	Capacity retention	Refs.
C@VO_2@V_2O_5	$ZnSO_4$	372 mAh g^{-1} (0.05 A g^{-1})	——	90.3 % after 2000 cycles at 5 A g^{-1}	1
$(NH_4)_{0.38}V_2O_5$	$Zn(CF_3SO_3)_2$	465 mAh g^{-1} (0.1 A g^{-1})	151.1 Wh kg^{-1}	89.3 % after 100 cycles at 0.1 A g^{-1}	2
KNVO	$Zn(CF_3SO_3)_2$	464 mAh g^{-1} (0.1 A g^{-1})	——	90 % after 3000 cycles at 5 A g^{-1}	3
$Na_{0.33}V_2O_5$	$Zn(CF_3SO_3)_2$	367 mAh g^{-1} (0.1 A g^{-1})	——	93% after 1000 cycles at 1 A g^{-1}	4
$NH_4V_4O_{10}$	$Zn(CF_3SO_3)_2$	489 mAh g^{-1} (0.5 A g^{-1})	——	90% after 8000 cycles at 15 A g^{-1}	5
$Na_{0.58}V_2O_5{\cdot}0.11H_2O$	$Zn(CF_3SO_3)_2$	540 mAh g^{-1} (0.2 A g^{-1})	——	92.1% after 100 cycles at 1 A g^{-1}	6
NVO-rGO/CNT	$Zn(CF_3SO_3)_2$	450 mAh g^{-1} (1 A g^{-1})	280.9 Wh kg^{-1}	83.1% after 1800 cycles at 10 A g^{-1}	7
$K_{0.23}V_2O_5$	$Zn(CF_3SO_3)_2$	284 mAh g^{-1} (0.1 A g^{-1})	——	92.8% after 500 cycles at 2 A g^{-1}	8
$Ca_{0.25}V_2O_5{\cdot}nH_2O$	$ZnSO_4$	340 mAh g^{-1} (0.2 C)	267 Wh kg^{-1}	96% after 3000 cycles at 80 C	9
$Mg_{0.34}V_2O_5{\cdot}0{\cdot}.84H_2O$	$Zn(CF_3SO_3)_2$	353 mAh g^{-1} (0.05 A g^{-1})	——	97% after 2000 cycles at 5 A g^{-1}	10
$Mg_{0.19}V_2O_5{\cdot}0.99H_2O$	$Zn(CF_3SO_3)_2$	425 mAh g^{-1} (0.2 A g^{-1})	7 9	98.1% after 5000 cycles at 5 A g^{-1}	11
$Mg_{0.2}V_2O_5{\cdot}nH_2O$	$Zn(CF_3SO_3)_2$	346 mAh g^{-1} (0.1 A g^{-1})	——	83.7% after 10000 cycles at 5 A g^{-1}	12
$Zn_{0.25}V_2O_5{\cdot}nH_2O$	$ZnSO_4$	300 mAh g^{-1} (0.3 A g^{-1})	250 Wh kg-^{1}	82% after 1000 cycles at 4.5 A g^{-1}	13
$Zn_{0.3}V_2O_5{\cdot}1.5H_2O$	$Zn(CF_3SO_3)_2$	426 mAh g^{-1} (0.2 A g^{-1})	336 Wh kg^{-1}	96% after 20000 cycles at 10 A g^{-1}	14
$Mn_{0.26}V_2O_5{\cdot}nH_2O$	$ZnSO_4$	484 mAh g^{-1} (0.1 A g^{-1})	——	95% after 500 cycles at 1 A g^{-1}	15
$Ni_{0.22}V_2O_5{\cdot}0.94H_2O$	$Zn(CF_3SO_3)_2$	442 mAh g^{-1} (0.1 A g^{-1})	287 Wh kg^{-1}	99.8% after 1500 cycles at 10 A g^{-1}	16
$Zn_{0.25}(NH_4)V_2O_5{\cdot}H_2O$	$Zn(CF_3SO_3)_2$	367 mAh g^{-1} (0.1 A g^{-1})	244.3 W h kg $^{-1}$	84.6% after 1220 cycles at 1 A g^{-1}	17
$(NH_4)_{0.5}V_2O_5$	$ZnSO_4$	394 mAh g^{-1} (0.2 A g^{-1})	——	91.4% after 2000 cycles at 5 A g^{-1}	18
$Al_{0.2}V_2O_5$	$Zn(CF_3SO_3)_2$	448 mAh g^{-1} (0.1 A g^{-1})	327.1 W h kg^{-1}	61.4% after 5000 cycles at 5 A g^{-1}	19
$NH_4V_4O_{10}$	$Zn(CF_3SO_3)_2$	475 mAh g^{-1} (0.4 A g^{-1})	332.25 W h kg^{-1}	90% after 2100 cycles at 5 A g^{-1}	20
NaNVO	$Zn(CF_3SO_3)_2$	468 mAh g^{-1} (0.1A g^{-1})	361 Wh kg^{-1}	99% after 2300 cycles at 2A g^{-1}	This work

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