Electrochemical performance and reaction mechanism investigation of V_2O_5 positive electrode material for aqueous rechargeable zinc batteries

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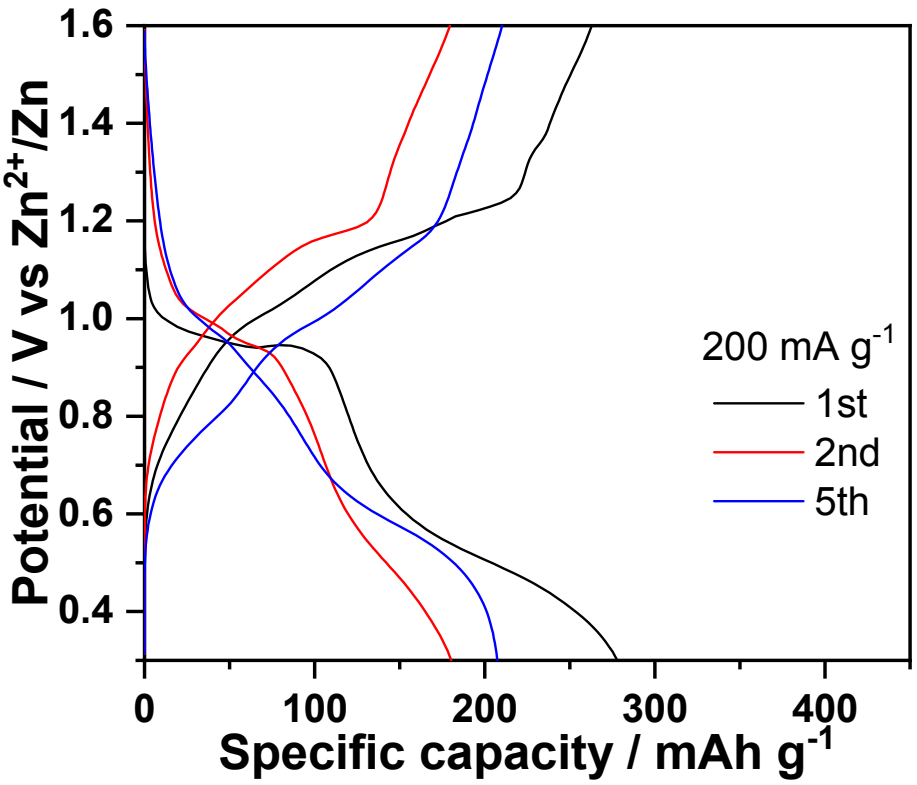
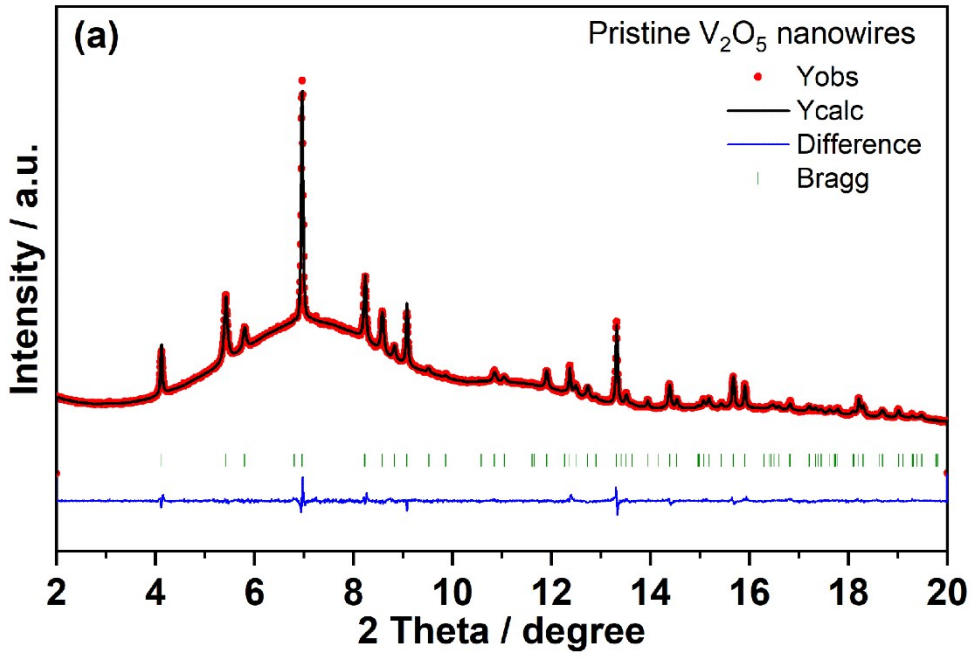
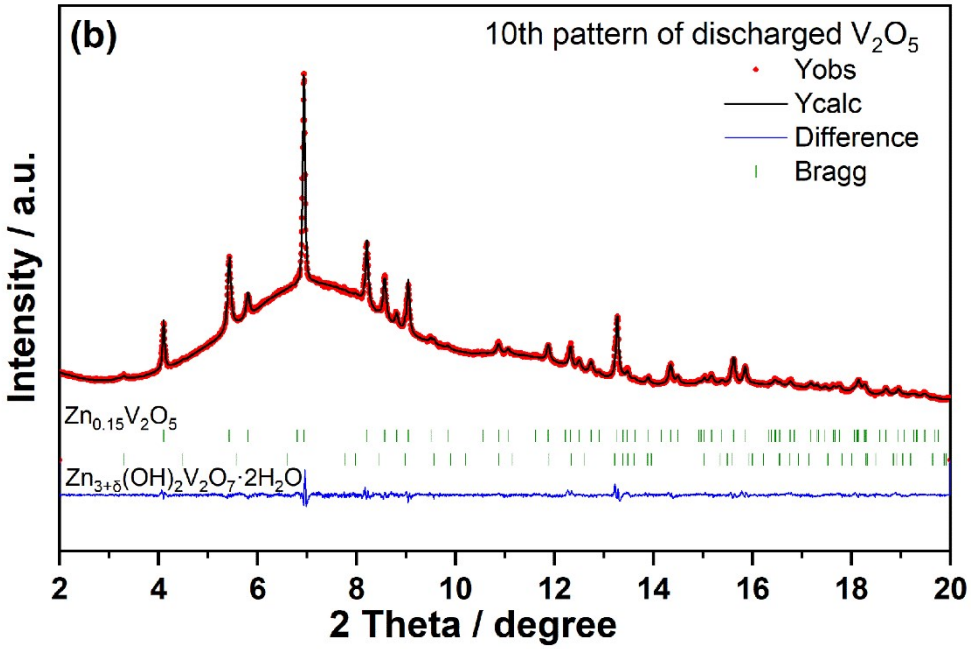
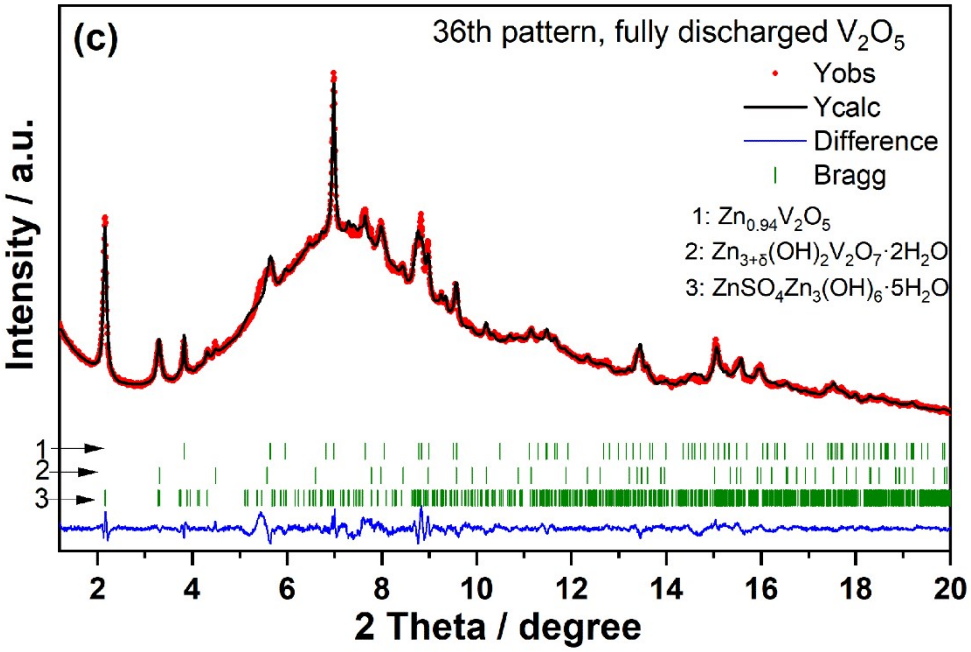


Figure S1 Discharge-charge profiles of V_2O_5 nanowires at 200 mA g^{-1} in 1 M $ZnSO_4$




(b)
10th pattern of discharged V_2O_5
Yobs
Ycalc
Difference
Bragg
Intensity / a.u.
$Zn_{0.15}V_2O_5$
$Zn_{3+\delta}(OH)_2V_2O_7{\cdot}2H_2O$
2
4
6
8
10
12
14
16
18
20
2 Theta / degree


(c)
36th pattern, fully discharged V_2O_5
Yobs
Ycalc
Difference
Bragg
1: $Zn_{0.94}V_2O_5$
2: $Zn_{3+\delta}(OH)_2V_2O_7{\cdot}2H_2O$
3: $ZnSO_4Zn_3(OH)_6{\cdot}5H_2O$
Intensity / a.u.
1
2
3
2
4
6
8
10
12
14
16
18
20
2 Theta / degree

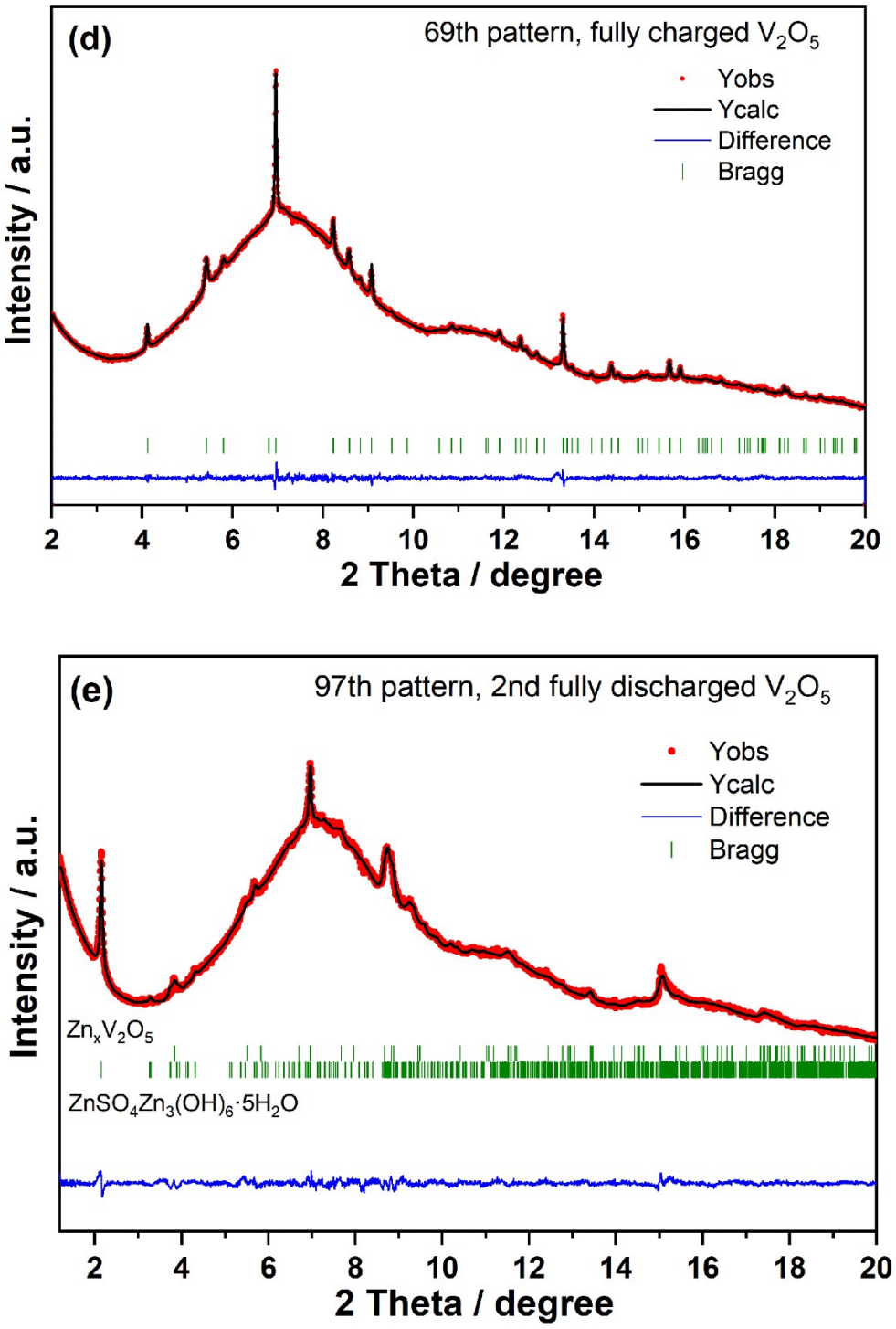


Figure S2 Rietveld refinement based on the pattern of the pristine V_2O_5 (a), discharged state in the beginning of Region II with the capacity of 44 mAh g^{-1} (10^{th} pattern, 1.02 V) (b), first fully discharged V_2O_5 electrode at 0.3 V (36^{th} pattern) (c), fully charged at 1.6 V(69^{th} pattern) (d), and 2^{nd} fully discharged V_2O_5 electrode at 0.3 V (97^{th} pattern) (e)

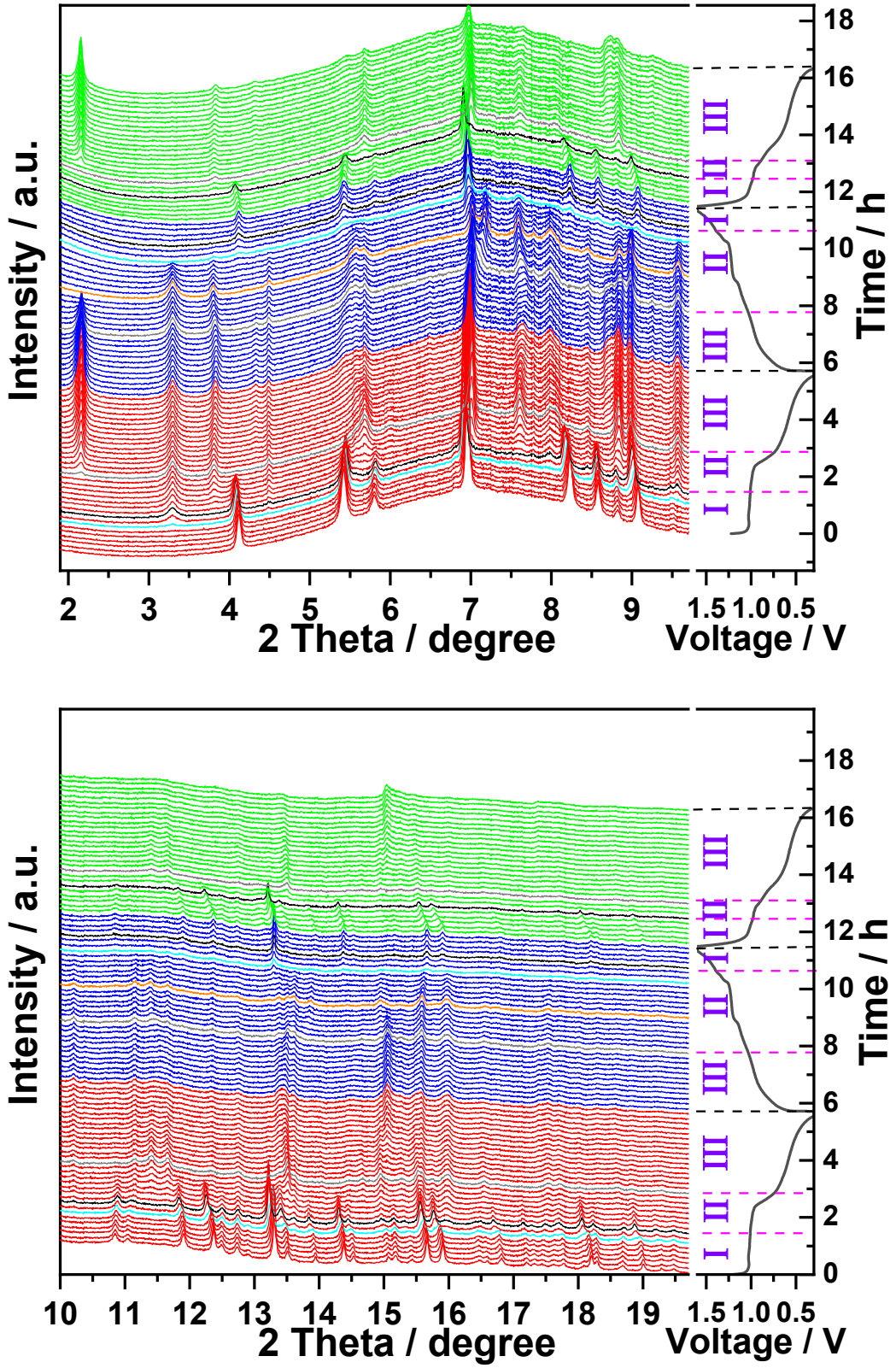


Figure S3 *In operando* synchrotron diffraction of V_2O_5 during the first one and half cycles and the corresponding voltage profile at a current density of 50 mA g^{-1}

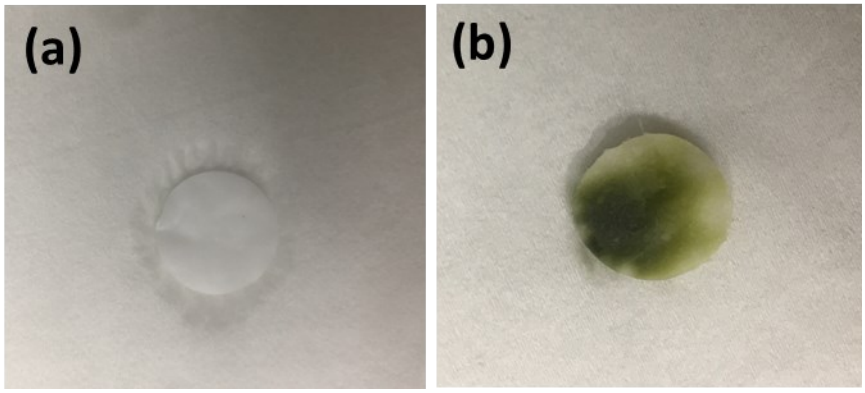


Figure S4 Images of separator from the 1st discharged V_2O_5 at 0.3 V (a) and the 1st charged V_2O_5 at 1.6 V (b)

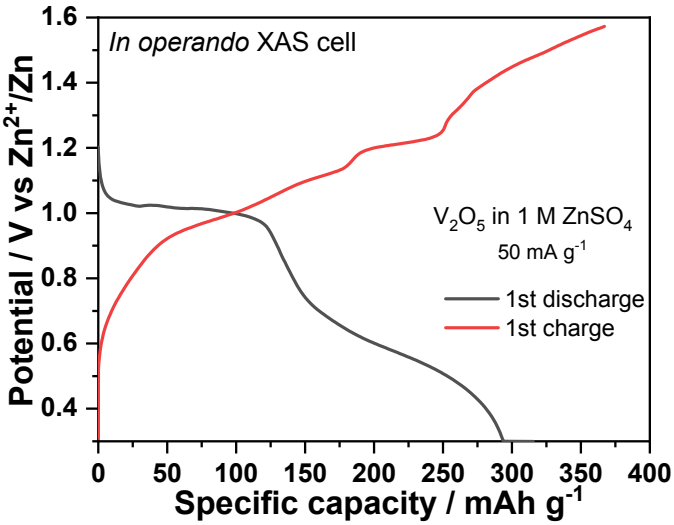


Figure S5 Discharge-charge profiles of V_2O_5 in 1 M $ZnSO_4$ electrolyte for *in operando* XAS (50 mA g^{-1})

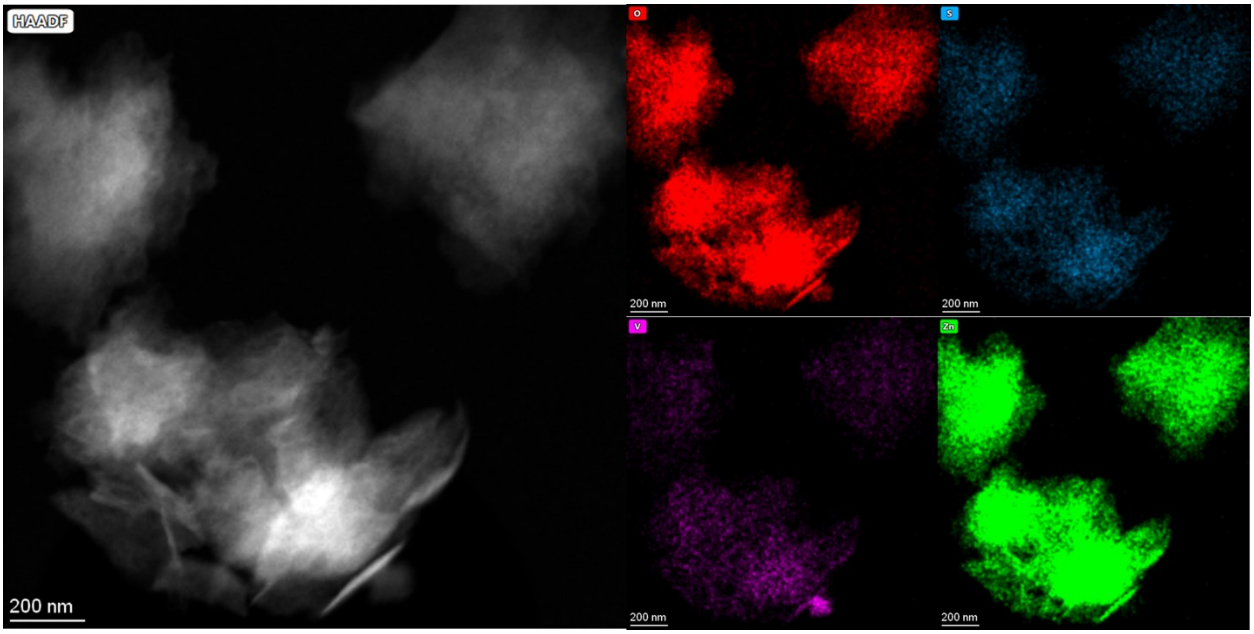


Figure S6 STEM-HAADF EDX mapping of O (red), S (blue), V (magenta), and Zn (green) for the 1st discharged V_2O_5

Table S1 Raman vibrational wavenumbers and assignments for V_2O_5 and Zn electrodes

Samples	Wavenumbers / cm^{-1}	assignments
Pristine and charged V_2O_5	994	V-O(1) stretching mode
	700	V–O(2) stretching vibration
	528	V–O(4) stretching vibration
	484	V–O(3) bending vibration
	405 and 284	V-O(1) stretching and bending vibrations
	304	V–O(4) bending vibrations
	197	δ(O2-V-O2)
	145	δ(O3-V-O2)
Discharged V_2O_5	1129, 967, and 610	v_3, v_1, v_4 of SO_4^{2-} vibration in $ZnSO_4Zn_3(OH)_6 \cdot nH_2O$
	876 and 450	V-O and Zn-O vibration of $Zn_xV_2O_5$ and $Zn_3(OH)_2V_2O_7 \cdot 2H_2O$
Zn counter electrode	440 and 566	Zn-O vibration of $Zn_{1+x}O$ on the surface of Zn
	1129, 967, and 398	v_3, v_1, v_4 of SO_4^{2-} vibration in the $ZnSO_4Zn_3(OH)_6 \cdot nH_2O$