Support information for：Constructing ultra-stable and high-performance zinc-ion batteries through Mn doped vanadium oxide nanobelt cathode

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Experimental Section

Materials preparation: The $Mn_xVO_2\cdot0.2H_2O$ was prepared with a simple solvothermal method. The Solvothermal solution was prepared by dissolving 0.6g V_2O_5 powder and 1.2g $H_2C_2O_4$ powder into 20 mL of distilled water at 85 °C for vigorous stirring about 3 h until VOC_2O_4 (dark blue solution) was formed. Then 4.67 mL 30 % H_2O_2 was slowly added (this step reacts violently) and kept continuously stirring about 30 min to obtain a brown solution, then 16 mg $Mn(CH_3COO)_2\cdot4H_2O$ was finally added into above-mentioned solution to obtain the Mn-doped vanadium oxide solution and stirred for 10 min until it was totally dissolved. The mixture was then given a 60 mL ethanol addition, and stirring continued for 60 min. The created dark-green slurry was then put into a 100 mL Teflon-lined autoclave and heated to 170°C for 12 hours. The precipitate was then collected, carefully cleaned with ethanol and deionized water, and dried for 12 hours at 60°C.

We analyzed the samples with an X-ray diffractometer using Cu Kα radiation (λ = 0.1542 nm). In order to determine the morphology and microstructure of the samples, scanning electron microscopy (SEM, Hitachi-4800) and transmission electron microscopy (TEM, JEM-2100 PLUS) were carried out. Chemical bond valences and elemental compositions of the cathode material surface were measured using X-ray photoelectron spectroscopy (XPS). A Bruker D8 Advance diffractometer was used to measure ex-situ XRD patterns of the samples.

The calculations are implemented in Vianna Ab-initio Simulation Package

of density functional theory, which use projector augmented wave method[1]. The following valence electron configurations are used: $O(1S^2 2S^2 2P^4)$, $V((1S^2 2S^2 2P^6 3S^2 3P^6 4S^2 3d^3)$, $Mn(1S^2 2S^2 2P^6 3S^2 3P^6 4S^2 3d^5)$ and $Zn(1S^2 2S^2 2P^6 3S^2 3P^6 4S^2 3d^{10})$. We select generalized gradient approximation (PBE flavor) as exchange-correlation potential [2]. Brillouin zone integrations are used for geometry optimization and electronic structure calculations, performing on 2×2×3 k-meshes. The energy criterion, iterative solution of the kohn-sham equations is set to 10^{-5} eV. A cut –off energy of plane wave basis is performed 450 eV, which is decided to yield converged results. On the atoms, the residual force is set to 0.03 eV/Å. When it less than 0.03 eV/Å, the structures will be relaxed.

An active electrode was prepared by mixing acetylene black, polytetrafluoroethylene emulsion, and active materials in a weight ratio of 2:1:7. Then upon rolling the mixture into a uniform thickness, which was pressed onto conductive carbon paper with a diameter of 1 cm. The active materials were loaded at an average mass of 1.3 mg/cm^2. A solution of $Zn(CF_3SO_3)_2$ was used as the electrolyte. The electrochemical characteristics and electrochemical reaction kinetics analysis of the coin cells were tested using an electrochemical workstation (Bio-Logic VSP-300). Galvanostatic charge-discharge cycling was carried out using multichannel galvanostatic testers (Neware CT-4000).

TableS1. ICP test results

Sample label	Element label	Weight /g	volume ml	Dilution coefficient	Instrument reading mg/L	Sample concentration	Unit
Yan Chen	Mn	0.0546	50	50	0.448	20512.7365	mg/kg
Yan Chen	V	0.0546	50	50	11.4468	524120.7064	mg/kg
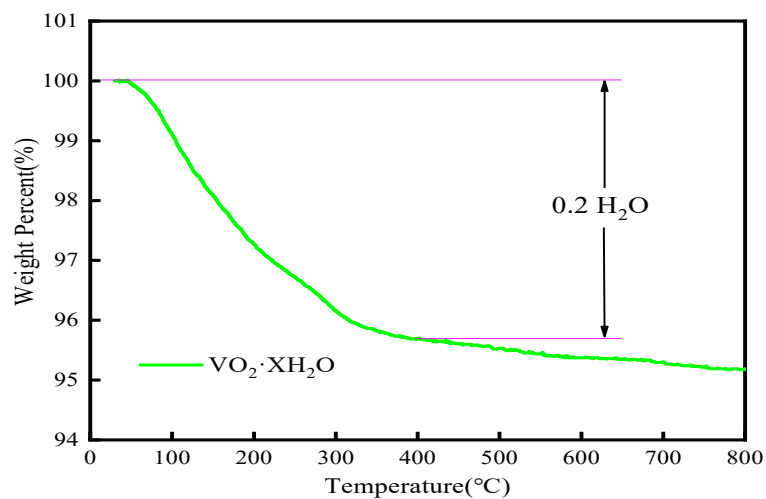
Figure S1. Thermogravimetric Curve of $VO_2 \bullet 0.2H_2O$
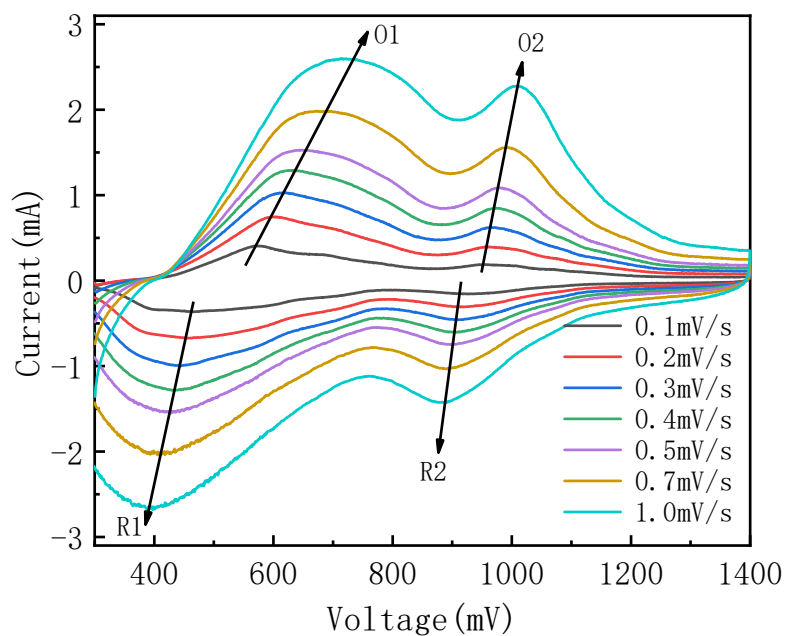
Figure S2. CV curves of $VO_2 \bullet 0.2H_2O$ at different scan rates
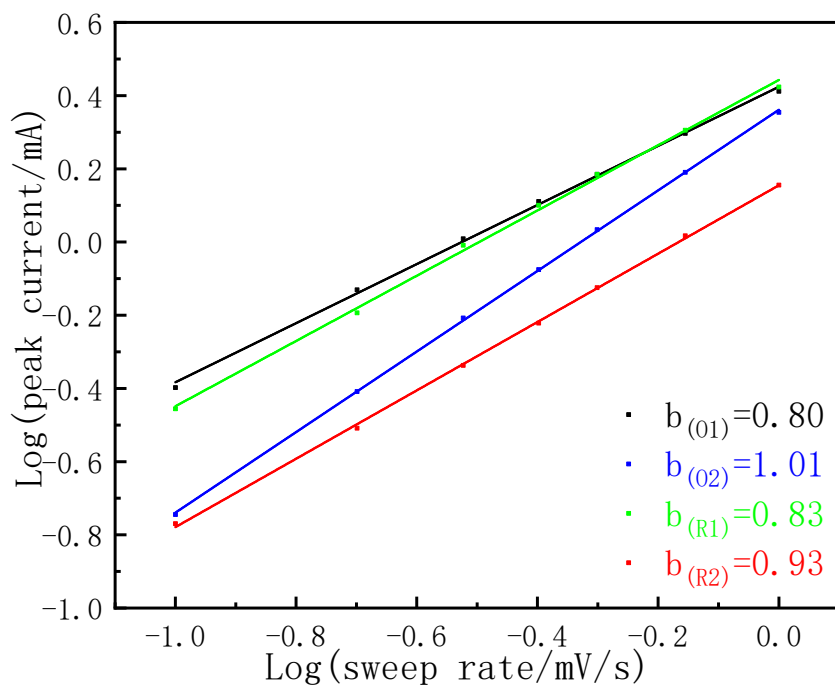
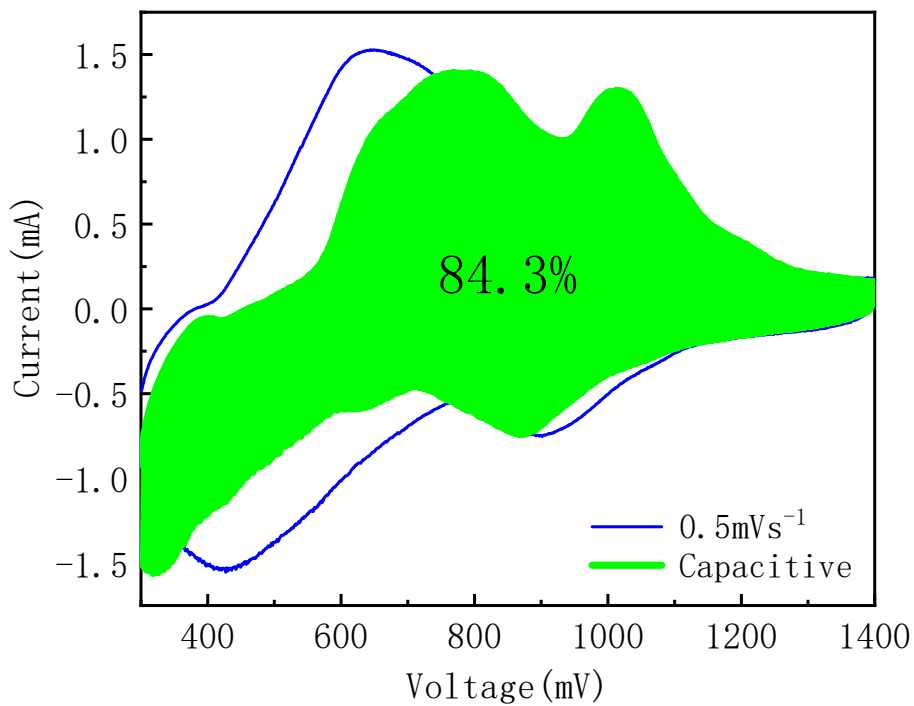**Figure S3.** Log (i, current) versus log (mV, scan rate) plots of $VO_2 \cdot 0.2H_2O$ at specific current.

Figure S4. The capacitive contribution ratio of $VO_2 \cdot 0.2H_2O$ at 0.5mVs^{-1} scan rates

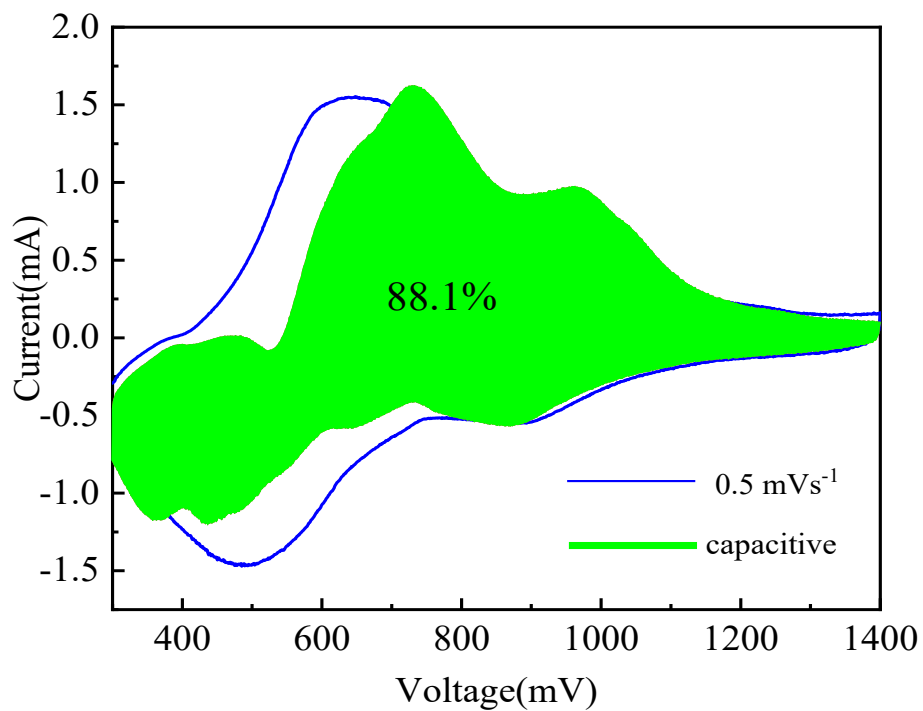**Figure S5.** The capacitive contribution ratio of $Mn_xVO_2 \cdot 0.2H_2O$ at $0.5mVs^{-1}$ scan rates

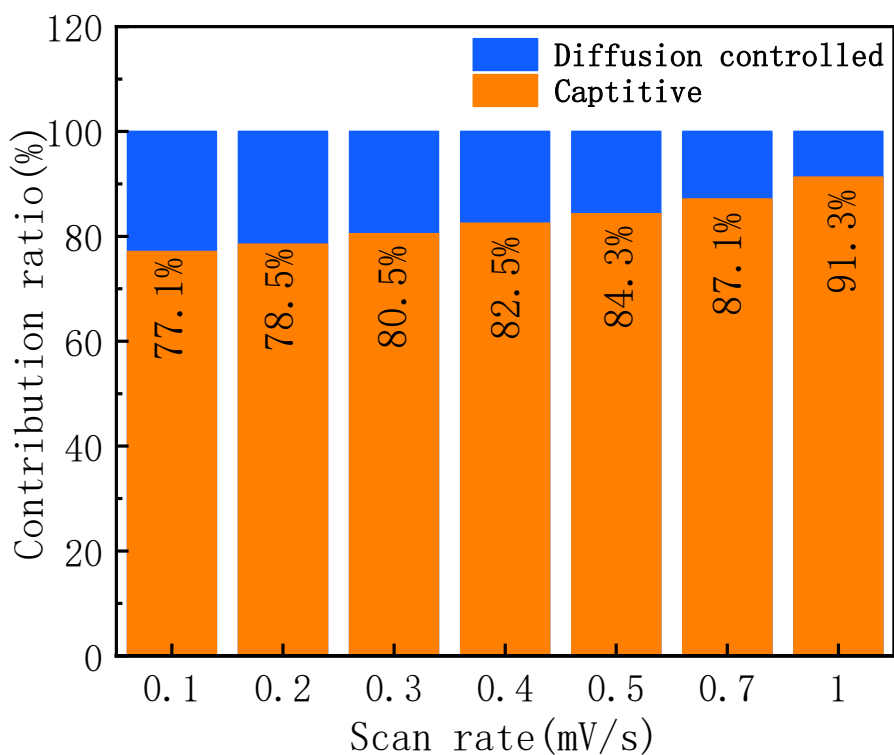**Figure S6.** The capacitive contribution ratio of $VO_2 \cdot 0.2H_2O$ at various scan rate

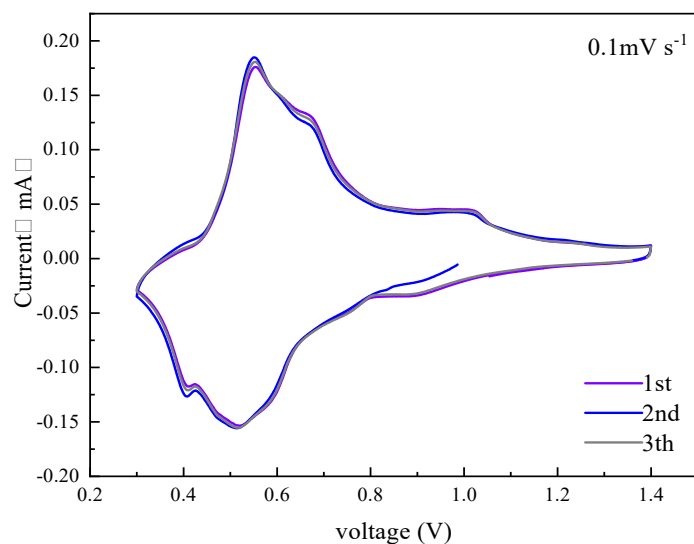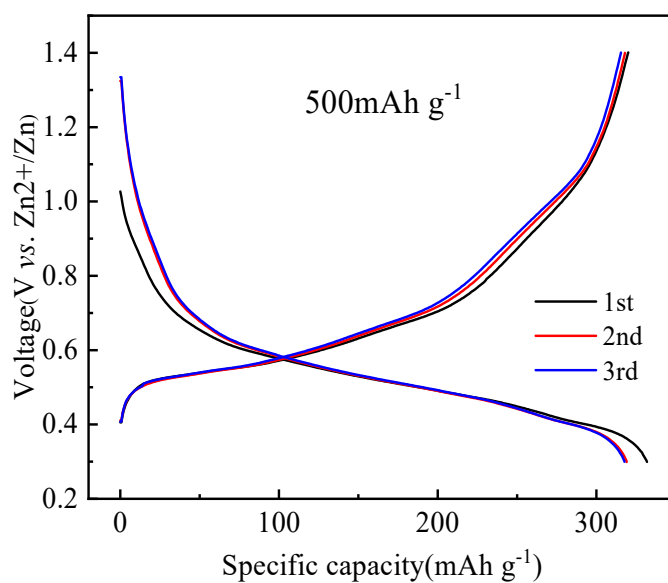**Figure S7.** CV curves of $VO_2 \cdot 0.2H_2O$ collected at a scan rate of 0.1 mV s^{-1}.

Figure S8. The first three discharge-charge profiles of $VO_2 \cdot 0.2H_2O$ at a current density of 500 mAg^{-1}.
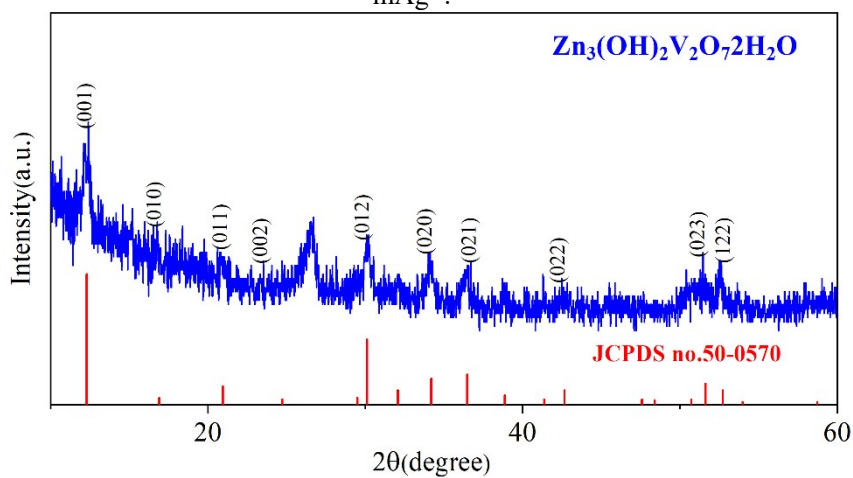

Figure S9. XRD patterns of $Mn_xVO_2 \cdot 0.2H_2O$ electrode sheet after 500 cycles

Table S2. Electrochemical impedance spectra of $Mn_xVO_2 \cdot 0.2H_2O$ and $VO_2 \cdot 0.2H_2O$

	$Mn_xVO_2 \cdot 0.2H_2O$ Pristine electrode	$VO_2 \cdot 0.2H_2O$ Pristine electrode	$Mn_xVO_2 \cdot 0.2H_2O$ 10 cycles	$VO_2 \cdot 0.2H_2O$ 10 cycles
Equivalent circuit diagram				
R2(Ω)	9.68	18.96	36.52	67.14
R1(Ω)	2.23	2.76	2.14	2.21

Table S3. The integral of the ICOHP

COHP# Zn- $Mn_{0.04}VO_2$	atom	atom	distance	ICOHP
Spin up	V17	O89	2.20497	-1.96883
Spin down	V17	O89	2.20497	-2.02170

COHP# Zn-VO_2	atom	atom	distance	ICOHP
Spin up	V15	O87	2.08418	-1.77492
Spin down	O15	V87	2.08418	-1.83334

Reference

(1) Enkovaara, J.; Rostgaard, C.; Mortensen, J. J.; Chen, J.; Dułak, M.; Ferrighi, L.; Gavnholt, J.; Glinsvad, C.; Haikola, V.; Hansen, H., Electronic structure calculations with GPAW: a real-space implementation of the projector augmented-wave method. *Journal of physics: Condensed matter* **2010,** *22* (25), 253202.

(2) Perdew, J. P.; Burke, K.; Ernzerhof, M., Generalized gradient approximation made simple. *Physical review letters* **1996,** *77* (18), 3865.