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Supporting Information

for *Small*, DOI: 10.1002/smll.201702551

High-Performance Aqueous Zinc–Ion Battery Based on Layered $H_2V_3O_8$ Nanowire Cathode

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High-performance aqueous zinc-ion battery based on layered $H_2V_3O_8$ nanowire cathode

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Experimental Section

Synthesis of $H_2V_3O_8$ nanowires: $H_2V_3O_8$ nanowires were synthesized by a facile, one-step hydrothermal method. First, 1.3 mmol V_2O_5 powder (0.237 g), 50 mL deionized (DI) water and 0.04 g poly(ethylene glycol) (PEG-4000) were successively added into 10 mL 30% hydrogen peroxide under vigorous stirring. Then the obtained solution was stirred continuously for one day at ambient conditions to achieve an orange solution. Afterwards, the mixed solution was sealed into a 100 mL Teflon lined stainless steel autoclave and hydrothermally treated at 180°C for 60 h. The products were collected and washed with DI water and ethanol alternately for three times. The dark-green powder was obtained after drying at 80°C for 10 h in air.

Materials characterization: The prepared samples were characterized by XRD (D8 Discover X-ray diffractometer with Cu Kα radiation), Raman spectroscopy (Renishaw INVIA), field emission scanning electron microscopy (FESEM, JSM-7100F) transmission electron microscopy (TEM), and XPS (Thermo Scientific Escalab 250Xi).

Electrochemical characterizations: For the preparation of electrodes, $H_2V_3O_8$ nanowires, acetylene black, and polyvinylidence fluoride (PVDF, 10 mg mL^{-1}), dissolved in N-Methyl pyrrolidone (NMP), were mixed in a weight ratio of 7: 2: 1 to obtain slurry. This mixture was then dispersed ultrasonically for about one hour until a dark homogeneous suspension was obtained. Later it was uniformly pasted on titanium foil, followed by drying at 70°C for 24 h, and finally cut into a circular disc of 10 mm in diameter with ~1.2 mg cm^{-2} active mass loading. For the fabrication of ZIBs, zinc metal was used as the anode, 3 M $Zn(CF_3SO_3)_2$ as electrolyte, stainless steel mesh as current collector and glass microfiber as the separator. A CR2016-type coin cell was assembled in the air atmosphere to evaluate the electrochemical performance on a LAND battery testing system (CT2001A). Cyclic voltammograms (CV) curves were recorded on a CHI600E electrochemical workstation. All of the tests were performed at room temperature.

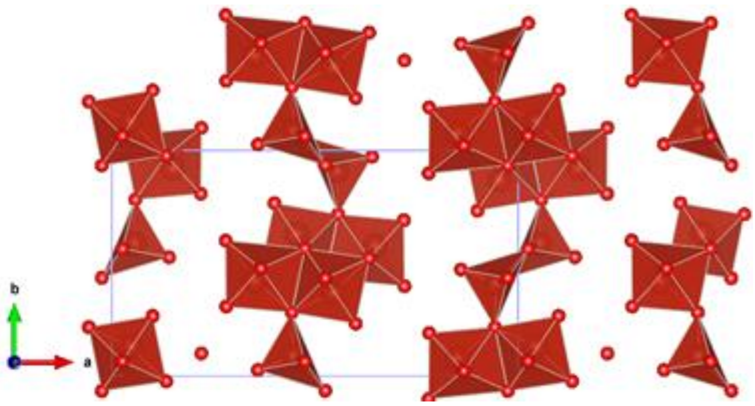

Figure S1. The crystal structure of $H_2V_3O_8$ nanowire.

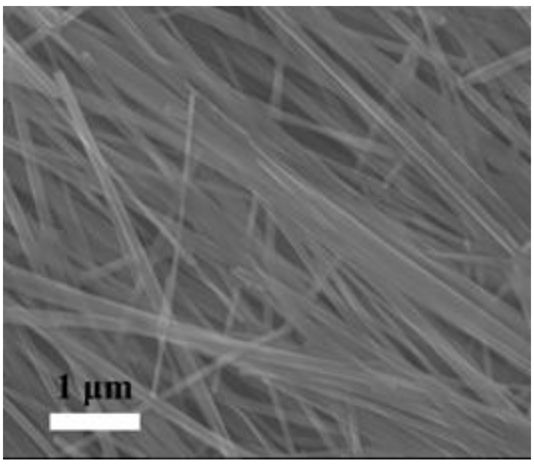

Figure S2. The SEM image of $H_2V_3O_8$ nanowire.

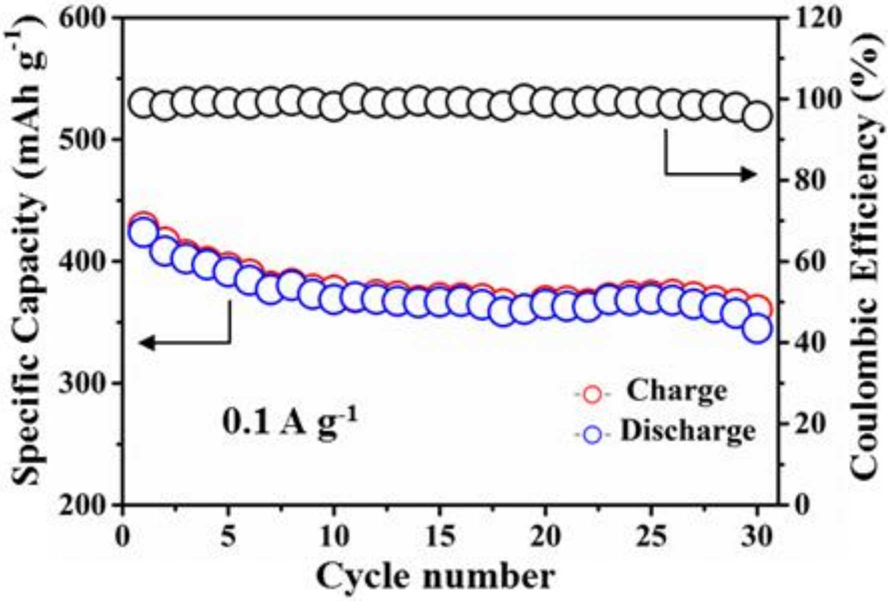

Figure S3. Cycling performance of Zn//$H_2V_3O_8$ battery at 0.1 A g^{-1}.

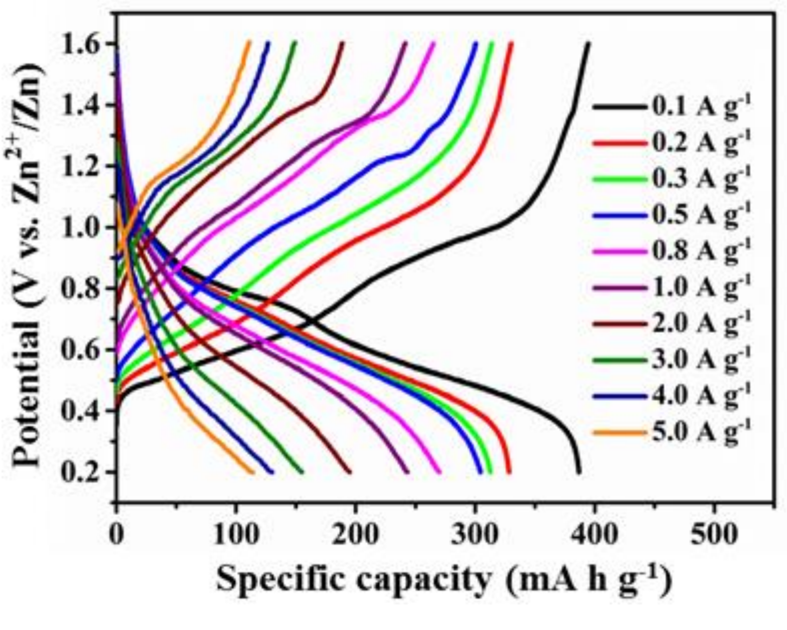

Figure S4. Charge/discharge profiles at different current densities.

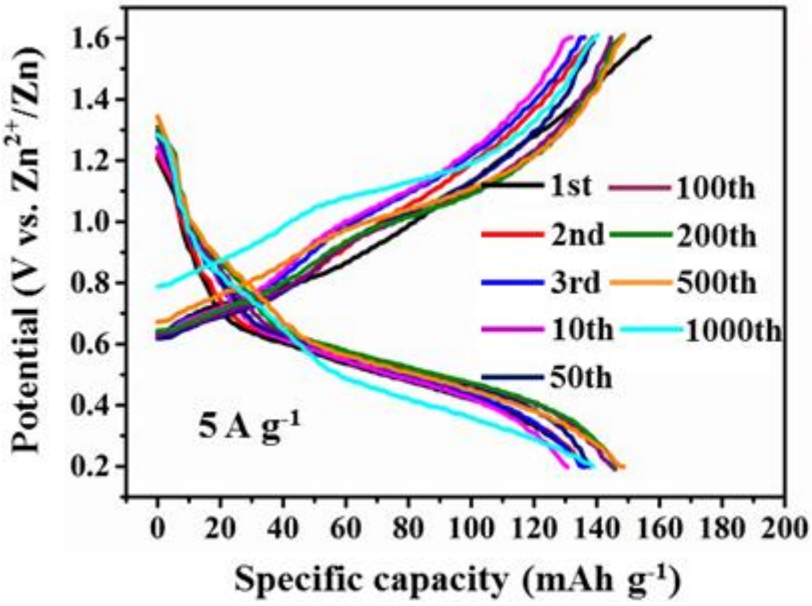

Figure S5. Charge/discharge profiles of different cycles at 5.0 A g^{-1}.

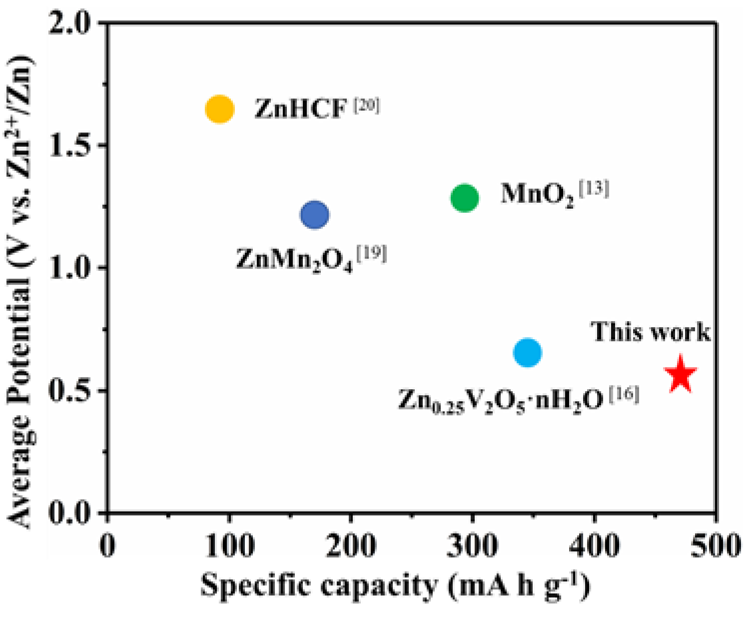

Figure S6. The comparison of Zn//$H_2V_3O_8$ to other related systems.

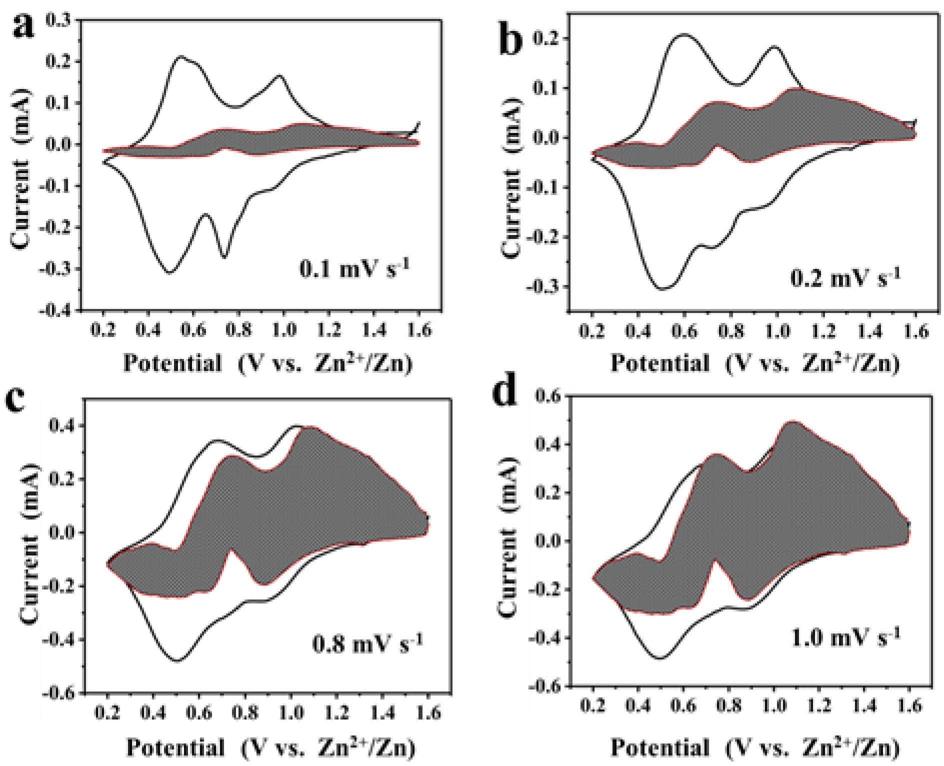

Figure S7. The contribution ratios of the capacitive capacities and diffusion-controlled capacities at (a) 0.1 mV s^{-1}, (b) 0.2 mV s^{-1}, (c) 0.8 mV s^{-1} and (d) 1.0 mV s^{-1}.

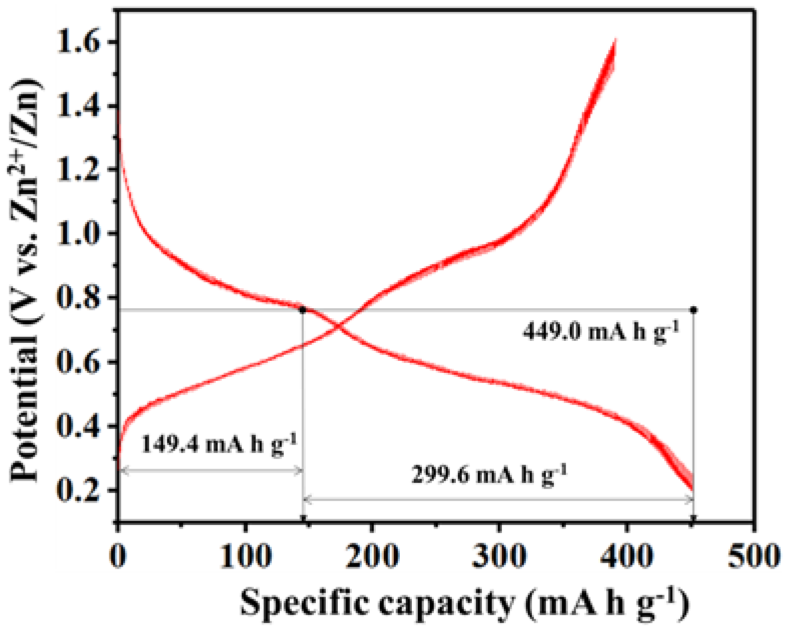

Figure S8. Charge/discharge curve of $Zn//H_2V_3O_8$ battery obtained during *GITT* measurement.

The intercalation of Zn ions into $H_2V_3O_8$ can be described by the following formula:

$$H_2V_3O_8 + 2x\,e^- + Zn^{2+} \rightarrow Zn_xH_2V_3O_8$$

The *x*-value can be quantified via the formula below:

$$Q = 2xF/3.6M$$

where Q refers to specific capacity (unit: mA h g^{-1}), and *x* is the number of moles of Zn ions involved in the electrochemical reaction, F is the faraday constant ($F = e \cdot N_A = 1.602176 \times 10^{-19}$ C × 6.02 × 1023 $mol^{-1} \approx 96500$ C mol^{-1}), and M is the molecular mass of active cathode material, 1 A h = 1 A × 3600 s = 3600 C.

Using the information listed above, *x* can be quantified to be 2.37.

Two pairs of sloping voltage plateaus in the charge/discharge curves obtained during *GITT* measurement are consistent with the redox peaks in the CV curves. And the multi-step mechanism of zinc ion intercalation can be described as below:

In the first step: $H_2V_3O_8 + 2xe^- + Zn^{2+} \rightarrow Zn_xH_2V_3O_8$ ($x = 0.79$)

In the second step: $Zn_xH_2V_3O_8 + 2ye^- + Zn^{2+} \rightarrow Zn_{x+y}H_2V_3O_8$ ($y = 1.58$)

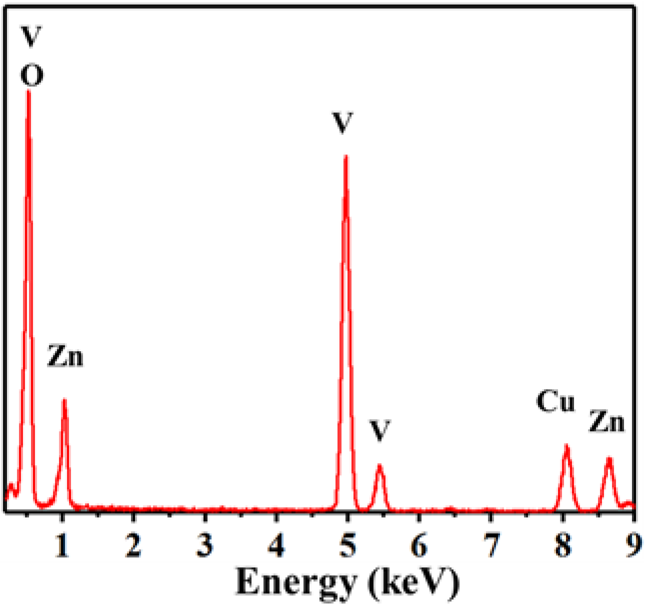

Figure S9. The EDX pattern of $H_2V_3O_8$ electrode at a full discharge state after three cycles.

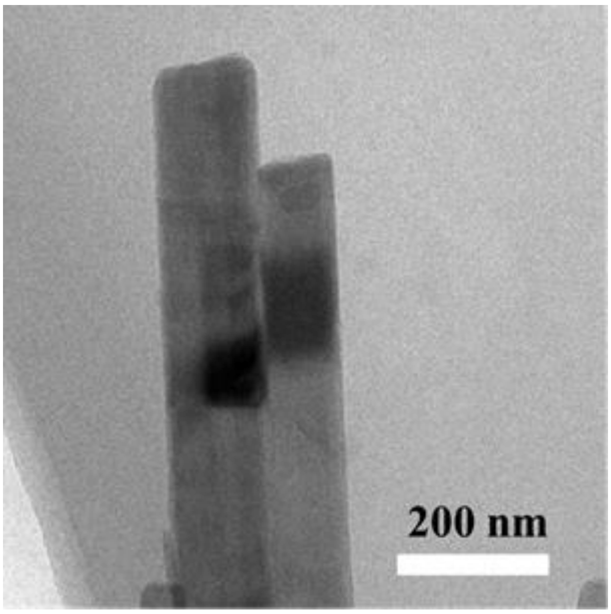

Figure S10. The TEM image of $H_2V_3O_8$ electrode after 100 cycles.