Supplementary material

Facile synthesis and electrochemical analysis of Zn-doped V_2O_5 anode materials for high-rate Li storage

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Table S1. Crystallite size calculation using Debye-Scherrer equation.

Sample	2θ (°)	hkl	FWHM (β) (°)	FWHM (β) (rad)	Crystallite size (nm)
V_2O_5	20.52	001	0.09	0.00157	89.8
	26.38	110	0.085	0.00148	96.2
Zn-V_2O_5	20.49	001	0.08	0.00140	100.6
	26.34	110	0.07	0.00122	116.7

To determine the particle size of V_2O_5 and Zn-V_2O_5 samples, we calculated the particle size of both samples from the XRD and TEM analysis results. The particle size of both samples from the XRD results based on the Debye-Scherrer equation can be calculated as follows [S1, S2]:

$$\mathrm{D} = \frac{k\lambda}{\beta \cos\theta}$$

Where D is the crystallite size (nm), k is a Sherrer constant (0.9), λ is the wavelength of the X-rays used (0.154 nm), β is the Full Width at Half Maximum (FWHM, radians), and θ is the peak position (radians). Based on the calculation results, the mean crystallite size of V_2O_5 was found to be lower, compared to that of Zn-V_2O_5.

[S1] A. O. Bokuniaeva, and A. S. Vorokh, "Estimation of particle size using the Debye equation and the Scherrer formula for polyphasic TiO_2 powder," Journal of Physics: Conference Series, vol. 1410, no. 1, pp. 012057, 2019.

[S2] S. Fatimah, R. Ragadhita, D. F. Al Husaeni, and A. B. D. Nandiyanto, "How to calculate crystallite size from x-ray diffraction (XRD) using Scherrer method," ASEAN Journal of Science and Engineering, vol. 2, no. 1, pp. 65-76, 2022.

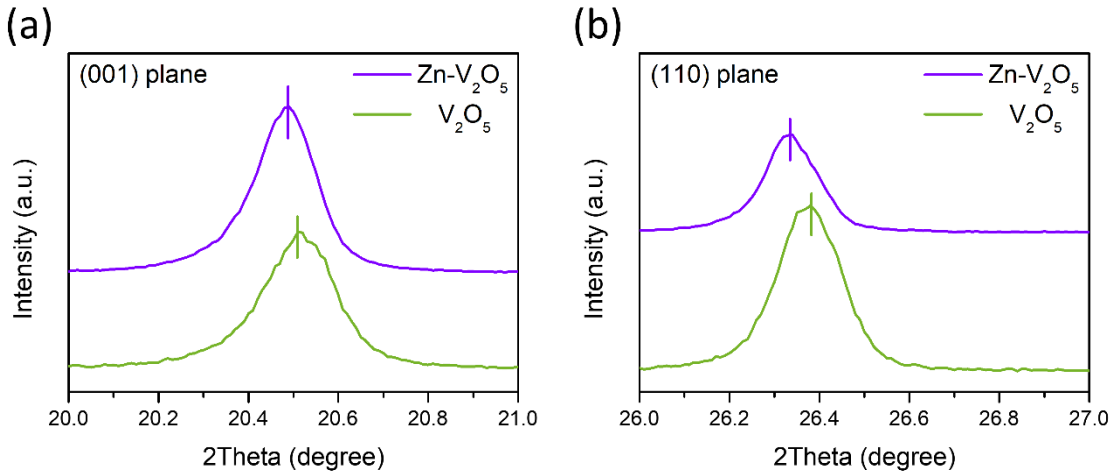

Figure S1. Enlarged XRD patterns of the Zn-V_2O_5 and V_2O_5 samples.

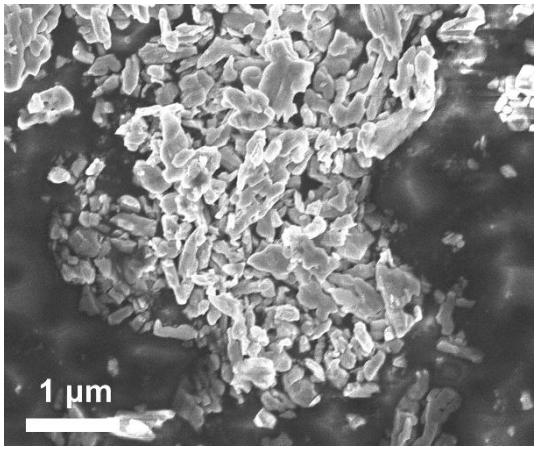

Figure S2. FE-SEM image of the V_2O_5 sample.

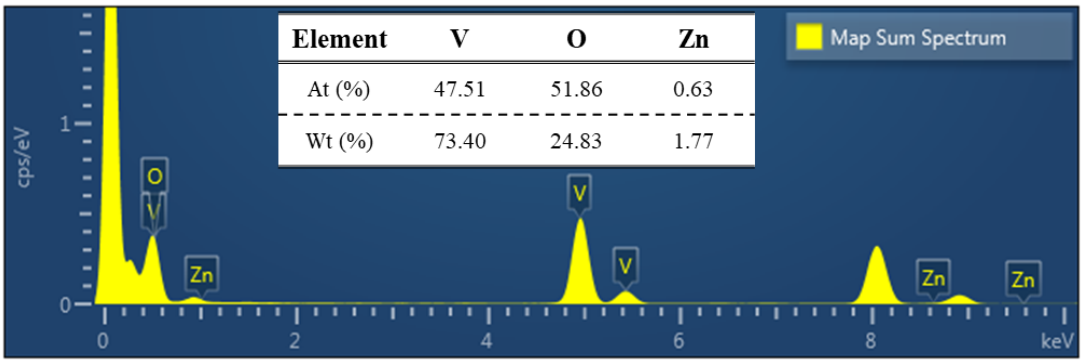

Figure S3. EDS results of the Zn-V_2O_5 sample.

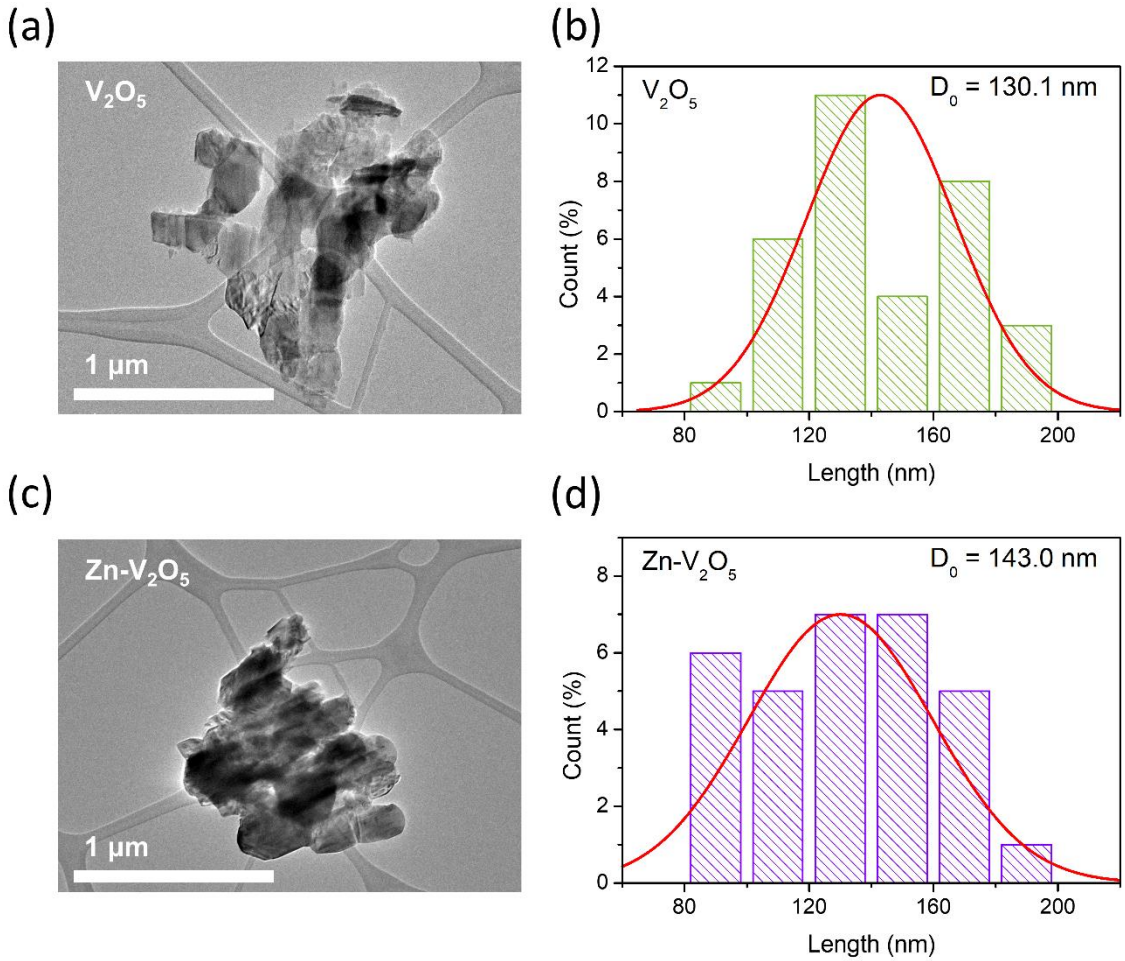

Figure S4. TEM images of the (a) V_2O_5 and (c) Zn-V_2O_5 samples. Particle size distribution plots obtained from TEM images of the (b) V_2O_5 and (d) Zn-V_2O_5 samples.

Figure S4 presents the TEM images and particle size distribution plots derived from the TEM images. The TEM images confirm the aggregation of nanoparticles in the order of hundreds of nanometers, forming larger particles in the micrometer range (Figure S4a and c). The mean particle sizes of the V_2O_5 and Zn-V_2O_5 samples were calculated to be 130.1 and 143.0 nm, respectively (Figure S4b and d). The particle size of V_2O_5 was observed to be smaller than that of Zn-V_2O_5, consistent with the results obtained from the XRD patterns. The mean particle sizes of the samples slightly differ from the values obtained using the Debye-Scherrer equation, likely due to measurement errors.

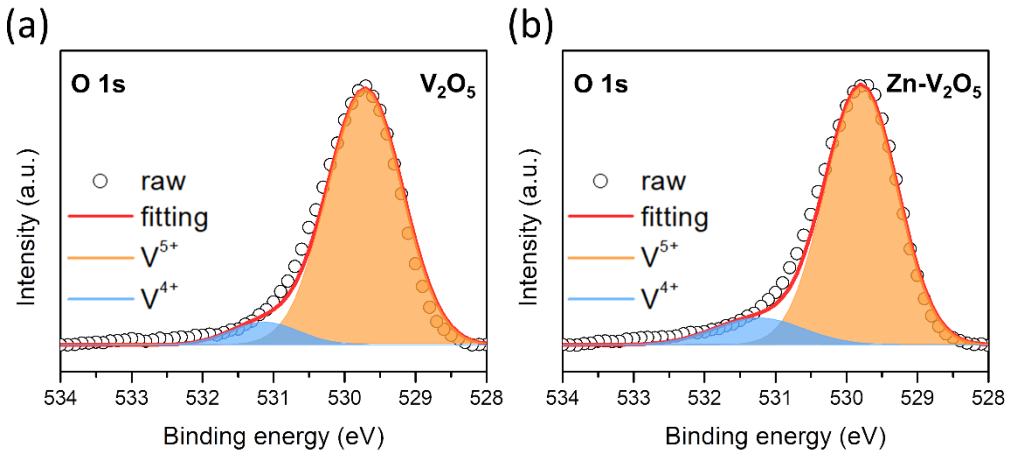

Figure S5. O 1s XPS core-level spectra for the (a) V_2O_5 and (b) Zn-V_2O_5 samples.

Table S2. Abundance ratio for the O valence states observed in the O 1s XPS spectra of the V_2O_5 and Zn-V_2O_5 samples.

Sample	Peak indexing	V^{5+}	V^{4+}
V_2O_5	Peak (eV)	529.8	531.2
	Area (%)	92.5	7.5
Zn-V_2O_5	Peak (eV)	529.9	531.2
	Area (%)	88.6	11.4

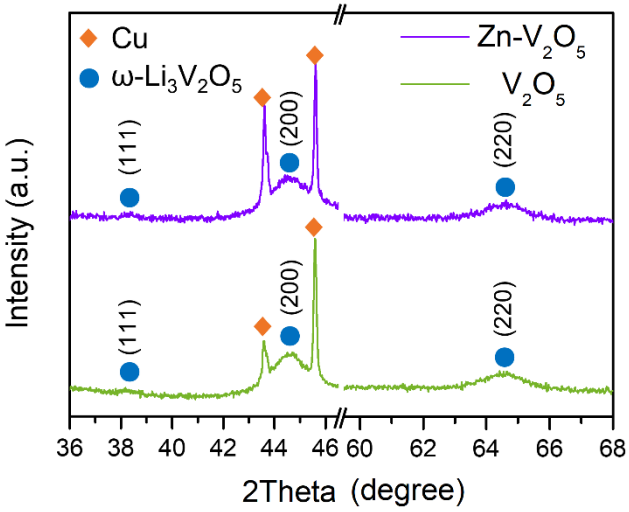

Figure S6. *Ex situ* XRD profiles of the V_2O_5 and Zn-V_2O_5 electrodes at a cutoff voltage of 1.9 V.

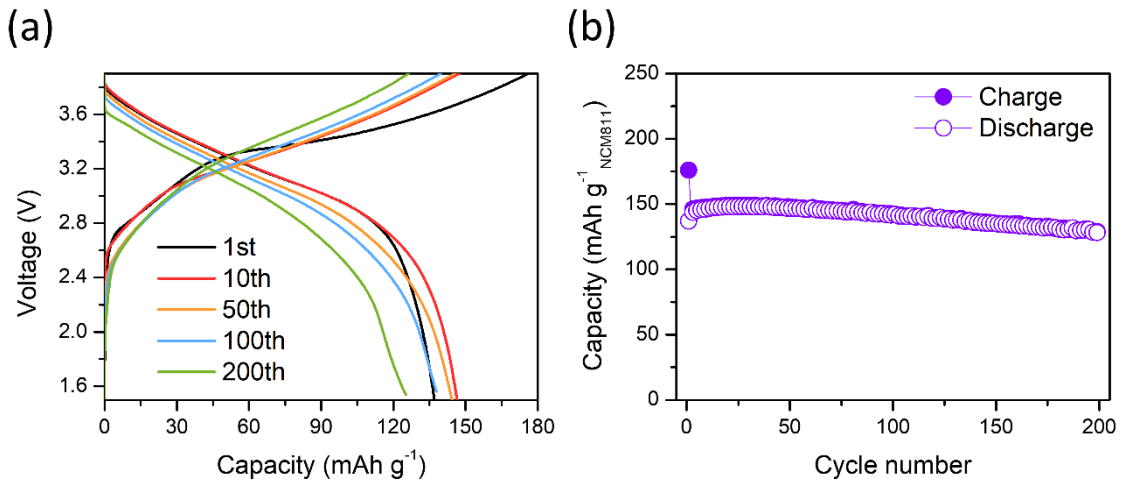

Figure S7. (a) Voltage profiles and (b) cycling performances of Zn-$Li_3V_2O_5$||NCM 811 full cell at 100 mA g^{-1}.

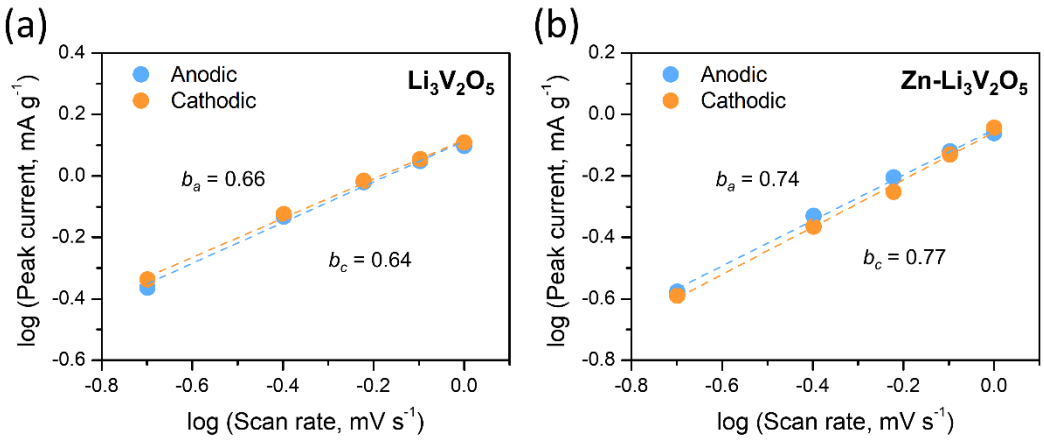

Figure S8. *b* values calculated from the log (Scan rate) vs. log (Peak current) curves.