

*Supporting Information for*

**NiSe/ZnSe heterojunctions derived from truncated rhombic  
dodecahedra for stable and high-power sodium-ion batteries**

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## **Experimental section**

### **Materials and Chemicals**

Nickel nitrate hexahydrate ( $\text{Ni}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ , 98%) , Zinc nitrate hexahydrate ( $\text{Zn}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ , 98%), Cetyltrimethylammonium bromide (CTAB, AR), 2-Methylimidazole (2-MeIM, 98%) were obtained from Aladdin, Methanol (99%) ,selenium powder (Se, 99%) were obtained from Macklin. All of the chemical reagents were used without further purification.

### **Materials Characterization**

The phase analysis and elemental composition of materials were measured by X-ray diffraction (XRD; D8ADVANCE), X-ray photoelectron spectroscopy (XPS; Thermo SCIENTIFIC ESCALAB 2560Xi). The morphology and microstructure of samples were characterized via Cold Field Emission Scanning Electron Microscope (SEM, Hitachi SU8000) and Transmission Electron Microscopy (TEM, TALOS F200X). In addition, the element content was determined by inductively coupled plasma atomic emission spectrometry (ICP-AES) (ICAP, 7400).

### **Preparation of Nickel-Zinc precursor**

A nickel-zinc organic ligand precursor exhibiting a truncated rhombic dodecahedral morphology was synthesized via a straightforward solvothermal approach. Briefly,  $\text{Ni}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$  and  $\text{Zn}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$  were utilized as metal sources at a 1:1 mass ratio. Cetyltrimethylammonium bromide (CTAB, 20 mg) was employed as a surfactant. Subsequently, 2-

methylimidazole (0.5 g) was added, and the mixture was dissolved in 60 mL of methanol. The solution was subjected to ultrasonic treatment until complete dissolution, followed by thorough stirring. The homogeneous mixture was then transferred to a 100 mL Teflon-lined autoclave and heated at 120 °C for 4 hours under solvothermal conditions. The resulting product was isolated by centrifugation, washed, and dried to yield a pale green powder, corresponding to the nickel-zinc precursor.

### **Preparation of NiSe/ZnSe**

The nickel-zinc precursor and selenium powder were separately loaded into different ceramic boats at a mass ratio of 1:3, and then placed in a quartz tube reactor (with the selenium powder placed upstream of the ventilation port and the precursor placed downstream of the ventilation port). Then, they were heated at a temperature of 500 °C under an Ar/H<sub>2</sub> atmosphere (5 vol% H<sub>2</sub>, 100-200 sscm) for 3 hours (heating rate: 2 °C/minute). The resulting powder after natural cooling was NiSe/ZnSe.

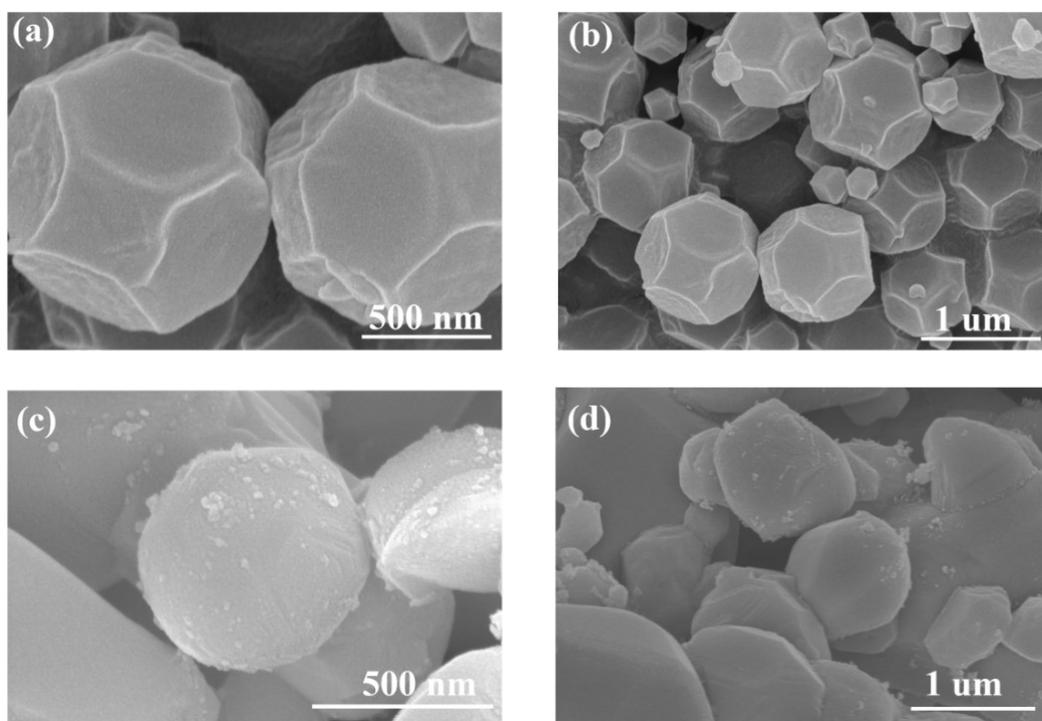
### **Electrochemical Measurements**

**For Half-cells:** The active materials (70 wt %), conductive carbon (Acetylene black, 20 wt %), and polyvinylidene fluoride (PVDF, 10 wt %) were uniformly dispersed into N-methylpyrrolidone (NMP) to obtain the slurry. Subsequently, the slurry was applied to the copper foil using a 200-micrometre squeegee and dried at 80°C for 12 hours. The active material loading was approximately 1 to 1.2 milligrams per square centimetre. The commercial Na<sub>3</sub>V<sub>2</sub>(PO<sub>4</sub>)<sub>3</sub> (NVP) (80 wt %), conductive carbon (Acetylene black, 10 wt %), and polyvinylidene fluoride (PVDF, 10 wt %) were uniformly dispersed into N-methylpyrrolidone (NMP) to obtain the slurry. Subsequently, the slurry was coated on the aluminum foil and dried at 80

°C for 12 h. The loading mass of the active materials is about 0.8~1 mg cm<sup>-2</sup>. The half-cells are assembled using the commercial sodium foil as the counter electrode, Whatman glass fiber membrane (GF/A) as the separator, and 1 M NaPF<sub>6</sub> dissolved in 1, 2-dimethoxyethane (DME) as electrolyte.

**For Full-cells:** To evaluate the performance of the NVP//NiSe/ZnSe full cell, NiSe/ZnSe was employed as the cathode and Na<sub>3</sub>V<sub>2</sub>(PO<sub>4</sub>)<sub>3</sub> as the anode, with an N/P ratio of 1.05. The electrolyte consisted of 1 M NaPF<sub>6</sub> in dimethyl ether (DME). Galvanostatic charge/discharge tests were carried out on a LAND (Wuhan, China) between 1 and 3.5 V vs. Na<sup>+</sup>/Na for full cells.

### Supplementary figures and tables



**Fig. S1** SEM morphologies of (a-b) Nickel-Zinc precursor; (c-d) NiSe/ZnSe

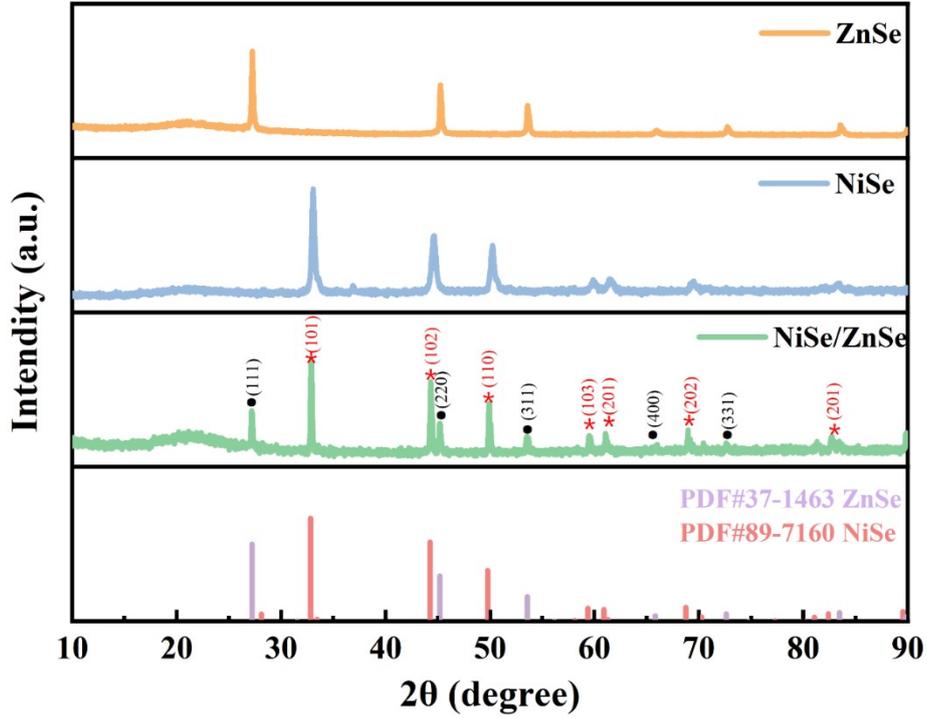


Fig. S2 XRD patterns of ZnSe · NiSe and NiSe/ZnSe

Table. S1 The Rietveld refinement results of NiSe/ZnSe

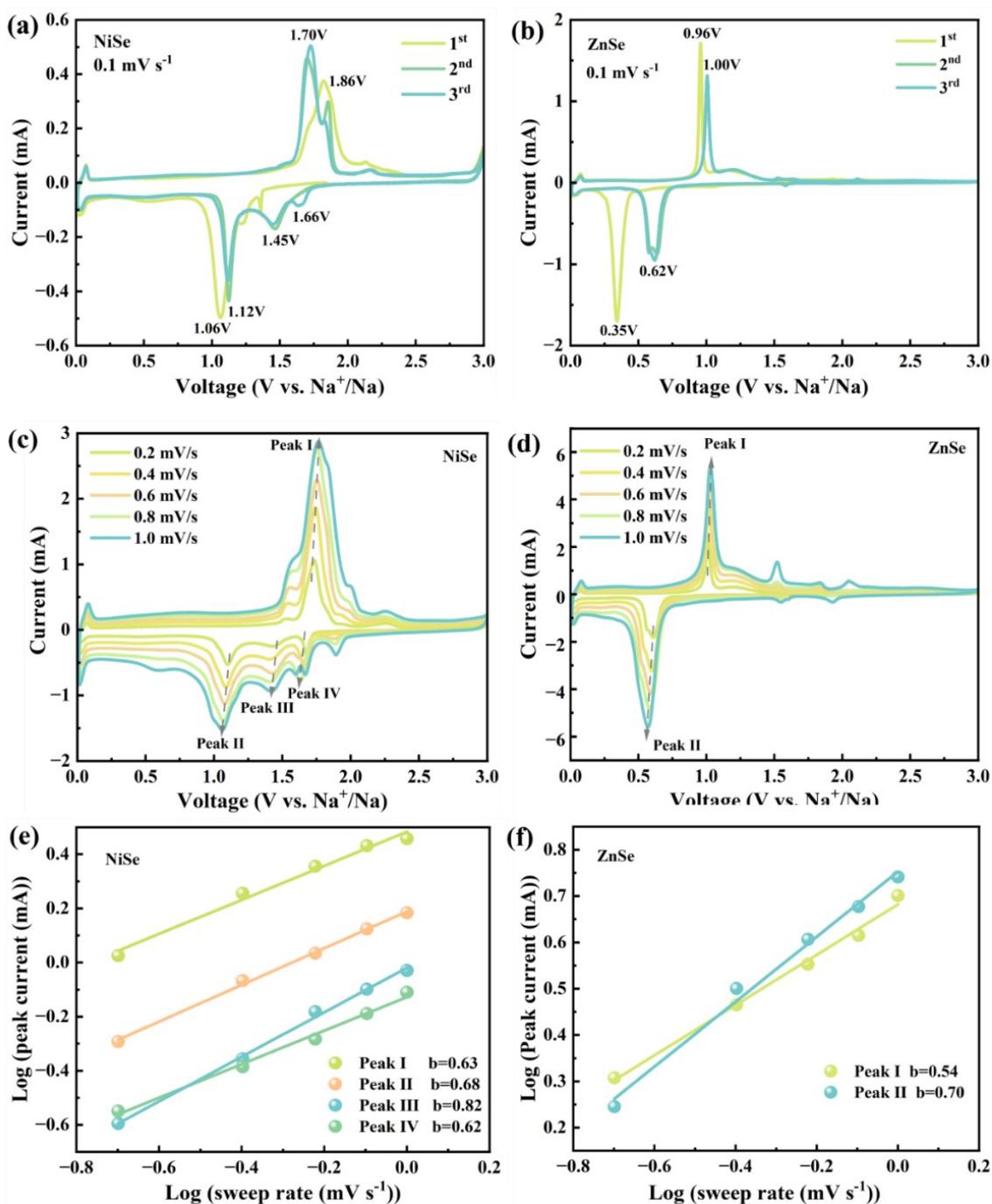
Composition	ZnSe	NiSe
Content	31.38%	68.62
JCPDF Card	37-1463	89-7160
space group	F-43m	P63/mmc
Crystal Cell	$a$ (Å)	5.66731
	$b$ (Å)	5.66731
	$c$ (Å)	5.66731
	$\alpha$ (°)	90
Data	$\beta$ (°)	90
	$\gamma$ (°)	90
	Volume (Å <sup>3</sup> )	182.025

**Table. S2** ZnSe atomic information based on XRD refinement results

Atom	Element	x	y	z	Biso	Occ	Mult
Zn1	Zn	0.25	0.25	0.25	1.611	0.042	4 None
Se1	Se	0	0	0	0.654	0.042	4 None

**Table. S3** NiSe atomic information based on XRD refinement results

Atom	Element	x	y	z	Biso	Occ	Mult
Ni1	Ni	0	0	0	1.611	0.683	2 None
Se1	Se	0.3333	0.6667	0.25	0.654	0.549	2 None



**Fig.S3** (a) the initial three CV curves of the NiSe electrode at  $0.1 \text{ mV s}^{-1}$  between 0.01 and 3.0 V; (b) the initial three CV curves of the ZnSe electrode at  $0.1 \text{ mV s}^{-1}$  between 0.01 and 3.0 V; (c) CV curves of NiSe at different scan rates from 0.2 to  $1.0 \text{ mV s}^{-1}$ ; (d) CV curves of ZnSe at different scan rates from 0.2 to  $1.0 \text{ mV s}^{-1}$ ; (e) corresponding  $\log(i)$  and  $\log(v)$  plots of NiSe; (f) corresponding  $\log(i)$  and  $\log(v)$  plots of ZnSe.

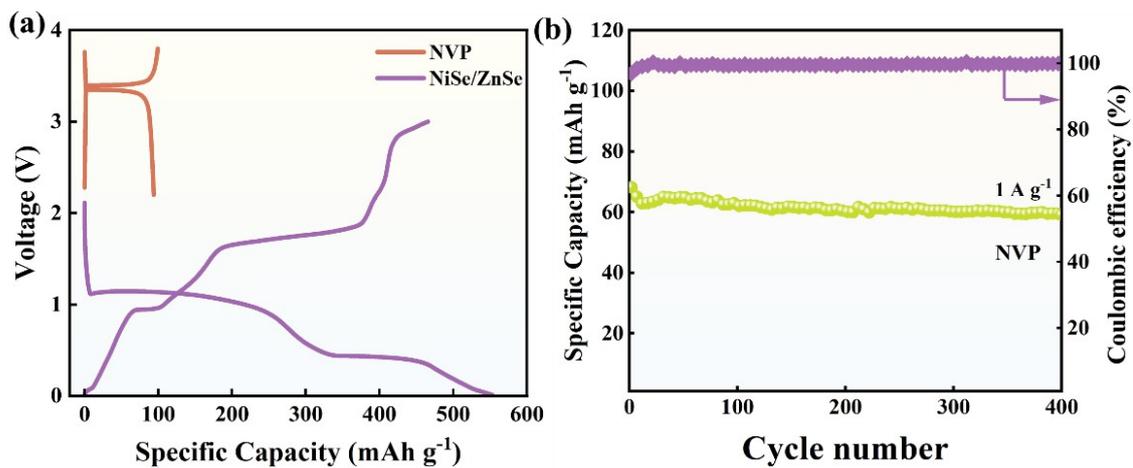


Fig. S4 (a) The GCD curve of NiSe/ZnSe anode and NVP cathode; (b) cycling stability at 1.0 A g<sup>-1</sup> of NVP

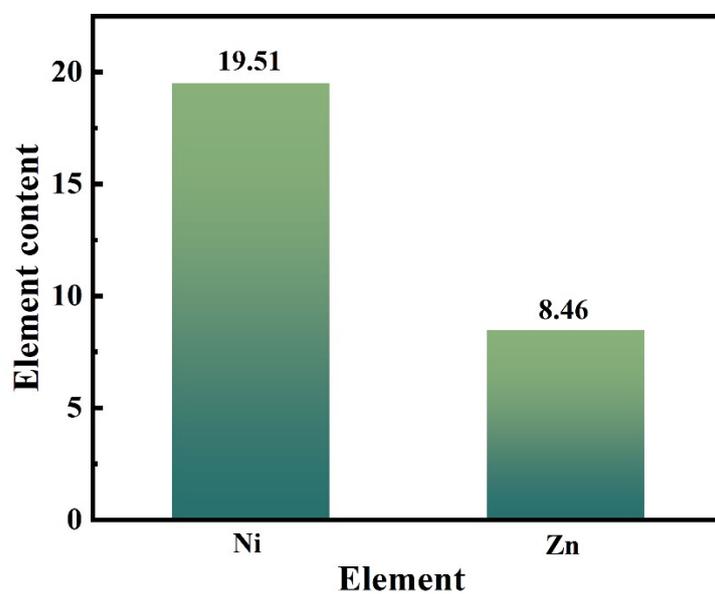


Fig. S5 ICP result of NiSe/ZnSe