Constructing VS_4-V_2CT_x heterojunction interface to realize ultra-long lifetime and high rate capability in sodium-ion batteries

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TGA analysis to calculate V_2CT_x content in VS_4-V_2CT_x

Assume that the amount lost during thermal decomposition of each component in the VS_4-V_2CT_x composite sample, and the amount decomposed when the components are pure substances remain constant. At this point we assume that the content of V_2CT_x and VS_4 in the composite sample is X and Y respectively, thereby setting out the following system of equations:

$$X + Y = 100\%$$

$$X*25.61\% + Y*40.88\% = 37.54\%$$

Therefore, X=21.87% Y=78.13%

The Na^+ ion diffusion (D_{Na^+}) for VS_4-V_2CT_x and VS_4 electrodes is calculated according to the following equation:

$$D_{Na^+} = 0.5(RT/AF2C\sigma)^2$$

where R = 8.314 J mol^{-1} K^{-1}, T = 303.15 K, A = 1.54 cm^2, F = 9.6486 × 10^4 C mol^{-1} , C ≈ 2 × 10^{-2} mol cm^{-3} , σ represents the Warburg impedance coefficient can be obtained from the following equation:

$$Z_{re} = R_e + R_{ct} + \sigma\omega^{-1/2}$$

The σ_w of the two electrodes are obtained by fitting in Figure S6 (b).

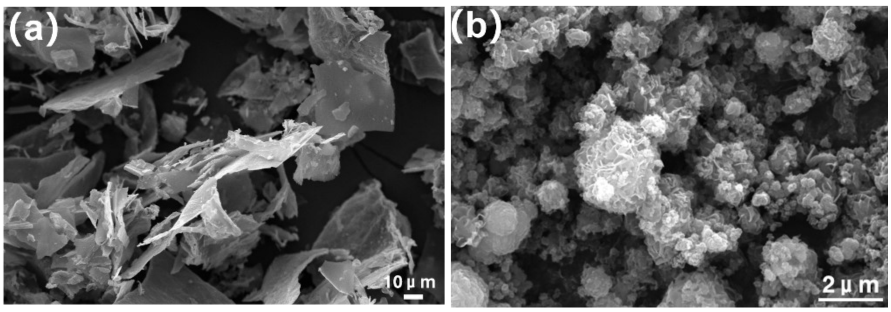

Figure S1. (a) SEM image of V_2CT_x, and (b) SEM image of VS_4;

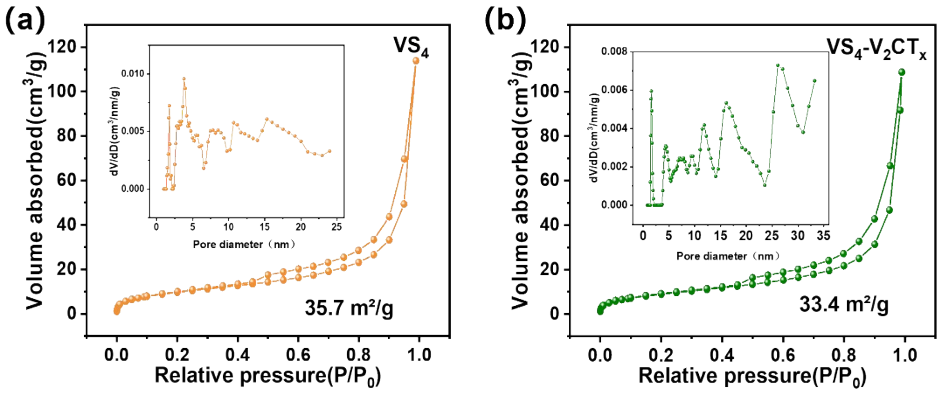

Figure S2 (a) Nitrogen adsorption–desorption isotherm of the VS_4 and (b) VS_4-V_2CT_x composites, the inset in (a) (b)shows the corresponding pore size distribution plot.

Table S1 BET data and pores data for VS_4 and VS_4-V_2CT_x

Material	BET surface (m^2g^{-1})	DFT		
		Pore Volume ($cm^2\ g^{-1}$)	Surface area (m^2g^{-1})	Pore width (nm)
VS_4	35.7	0.10	24.0	3.8
VS_4-V_2CT_x	33.4	0.11	27.8	26.1

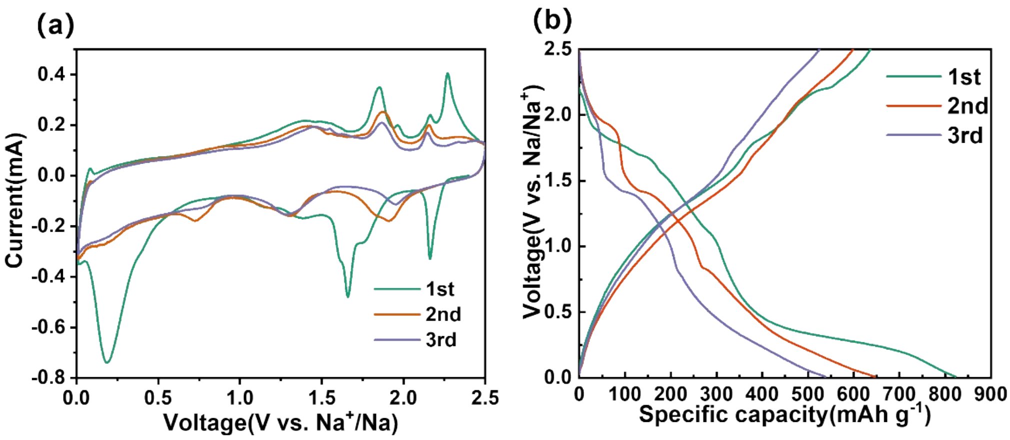

Figure S3. (a) CV curves of the VS_4 electrode and (b) Galvanostatic charge/discharge curves of VS_4

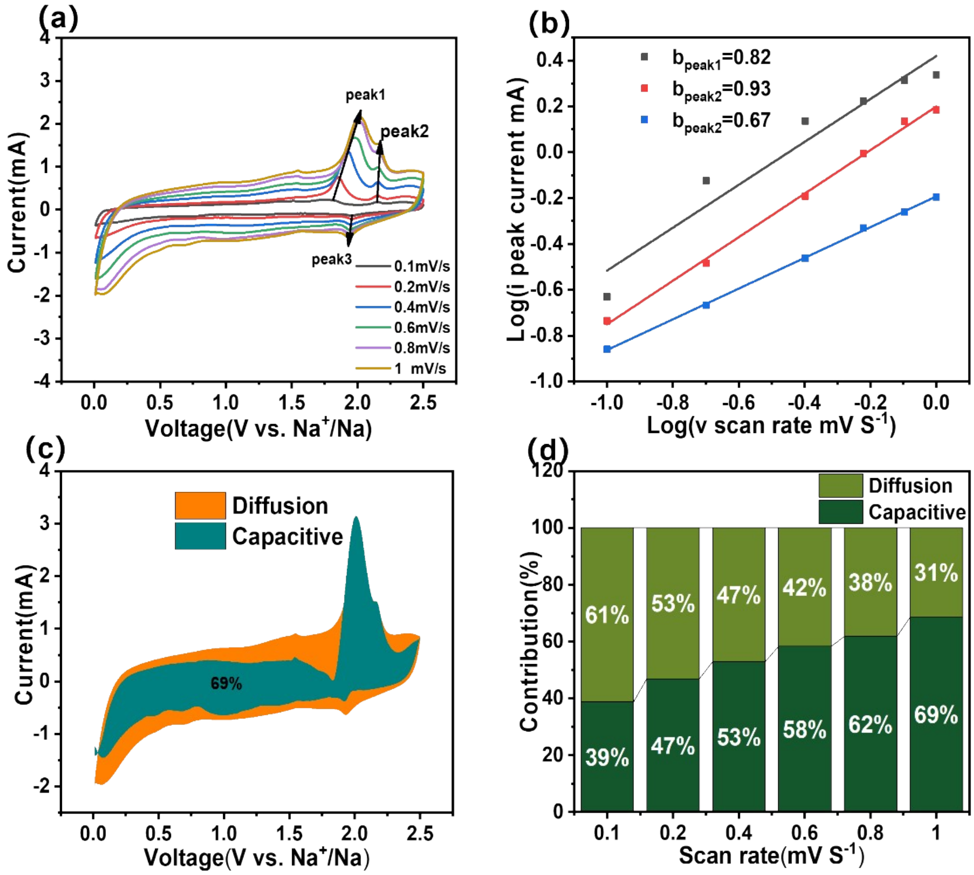

Figure S4. (a) CV curves of the VS_4 electrode tested at different scan rates; (b) relationship between log i and log ν plots of the VS_4 electrode; (c) capacitance contribution at 1.0 mV s^{-1} for the VS_4 electrode; (h) capacitance contribution of the VS_4 electrode at different scan rates

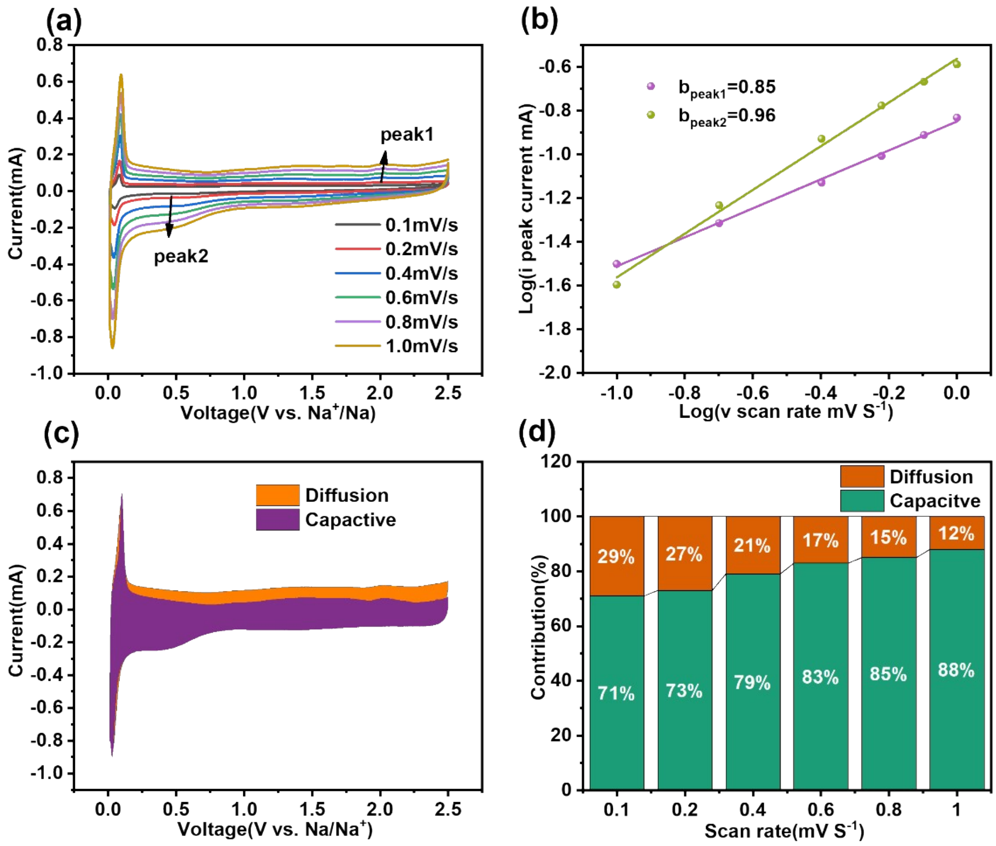

Figure S5. (a) CV curves of the V_2CT_x electrode tested at different scan rates; (b) relationship between log i and log ν plots of the V_2CT_x electrode; (c) capacitance contribution at 1.0 mV s^{-1} for the V_2CT_x electrode; (h) capacitance contribution of the V_2CT_x electrode at different scan rates

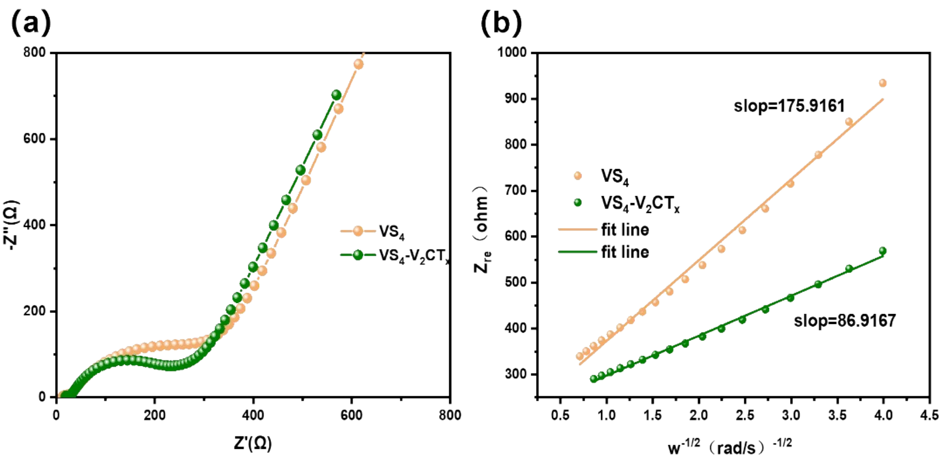

Figure S6. (a) The Nyquist plots and (b) linear fits in low-frequency regions of the VS_4-V_2CT_x and VS_4 electrodes after 100 cycles at discharge state.

Table S2 Electrochemical impedance parameters of the VS_4 and VS_4-V_2CT_x electrodes

Samples	R_e	R_f	R_{ct}	σ (Ω cm^2 $s^{-1/2}$)	D_{Na^+} (cm^2 s^{-1})
VS_4	11.01	18.25	295.4	175.9161	$5.22*10^{-6}$
VS_4-V_2CT_x	16.66	6.51	140.1	86.9167	$2.14*10^{-5}$

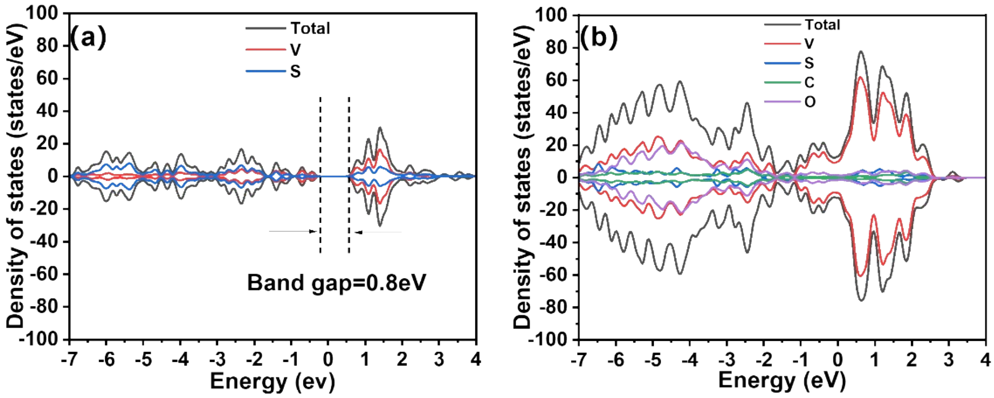

Figure S7. Total density of states of (a) VS_4 and (b) VS_4-V_2CT_x heterojunction.

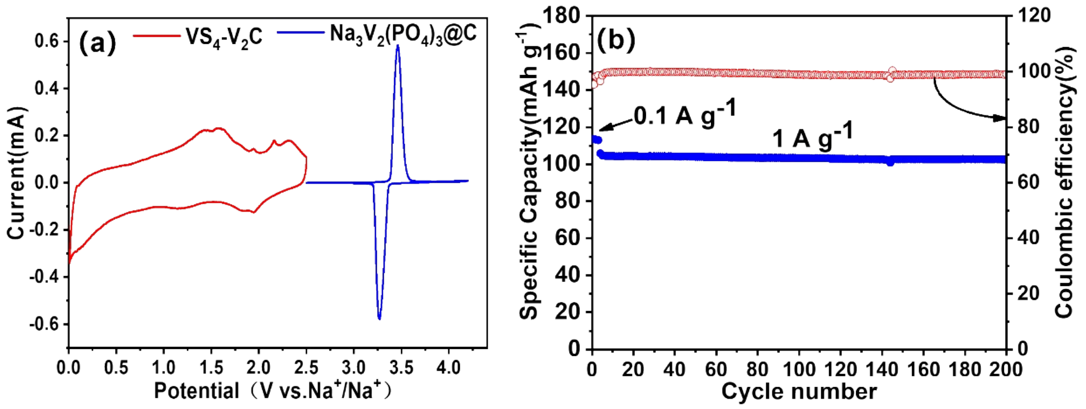

Figure S8. (a) CV curves of the VS_4-V_2C and $Na_3V_2(PO_4)_3$@C electrode at 0.1 mV s^{-1}; (b) Long cycling performance of $Na_3V_2(PO_4)_3$@C electrode at a current density of 1 A g^{-1} (0.1 A g^{-1} for the first three cycles);