

Supporting Information

Sulfide Cluster Vacancy Inducing an Electrochemical Reversibility Improvement of Titanium Disulfide Electrode

Material

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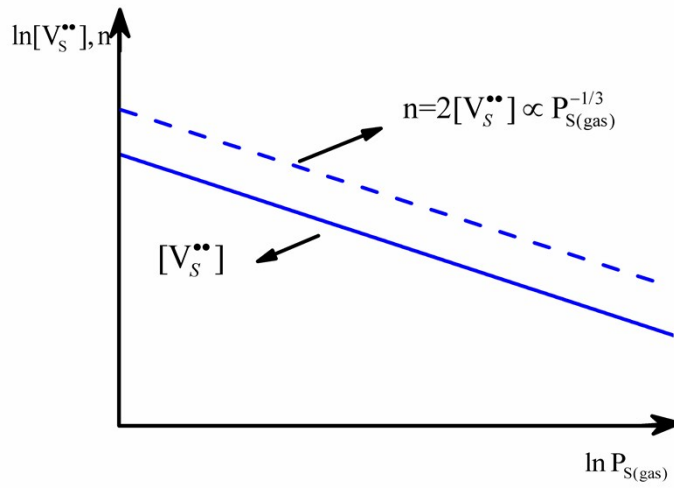


Fig. S1 A Plot of $\ln[n]/\ln [V_s^{..}] - \ln P_{S(gas)}$ (Brouwer diagramm)

The sulfur vacancies are denoted as $[V_s^{..}]$, partial pressure of sulfur is $P_{S(gas)}$ and n is free electron. According to the equilibrium constant of vacancy reaction and neutral condition, the relationship between sulfur vacancy concentration and partial pressure of sulfur can be shown in the Fig. S1.

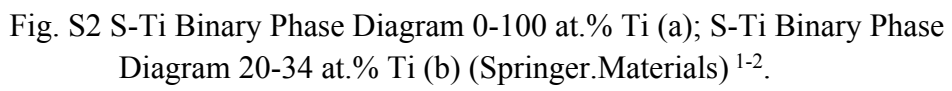


Fig. S2 S-Ti Binary Phase Diagram 0-100 at.% Ti (a); S-Ti Binary Phase Diagram 20-34 at.% Ti (b) (Springer.Materials)¹⁻².

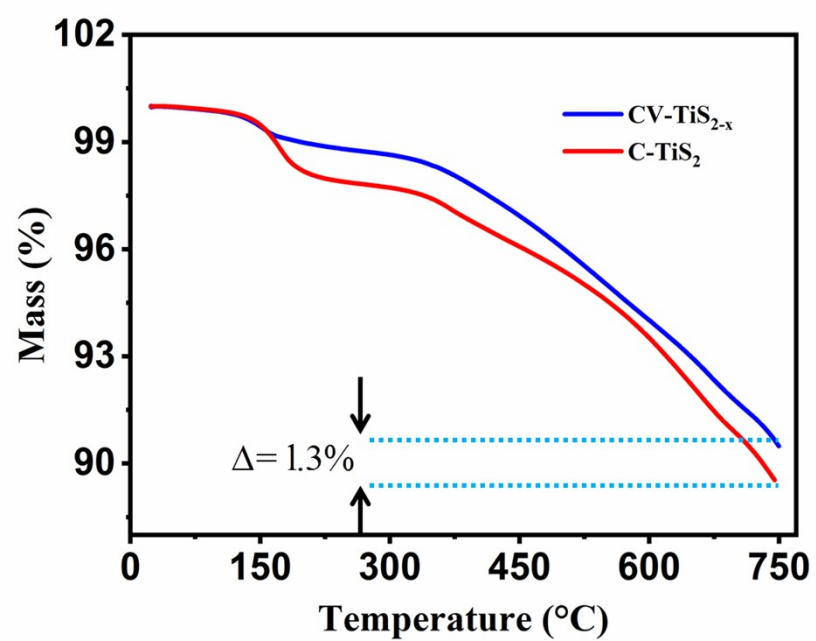


Fig. S3 TGA analysis of CV-TiS_{2-x} and C-TiS₂.

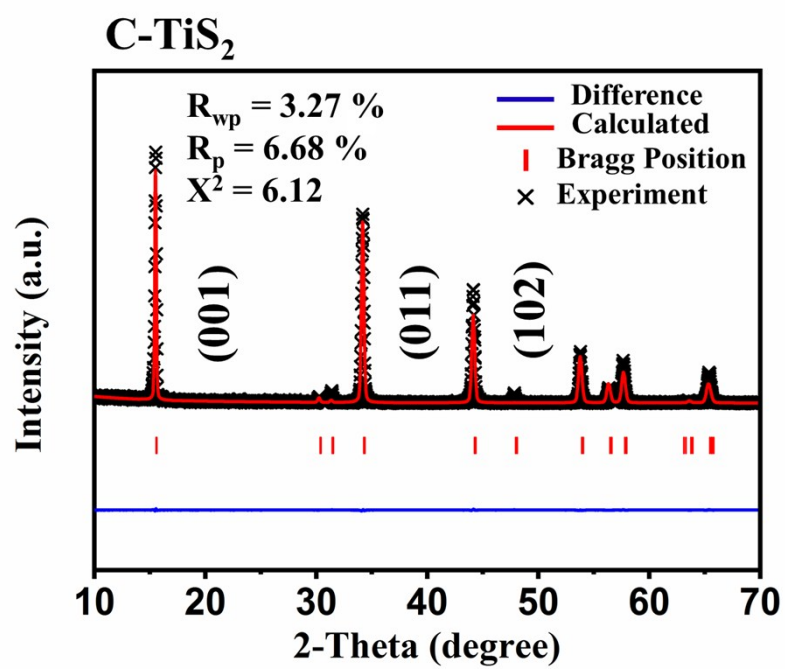


Fig. S4 The XRD pattern of C-TiS₂.

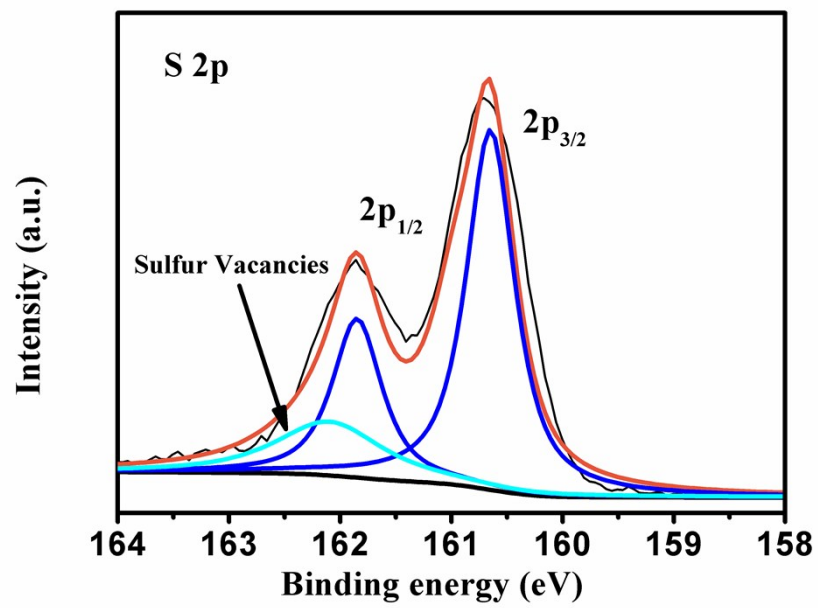


Fig. S5 S 2p XPS spectra regions for CV-TiS_{2-x}.

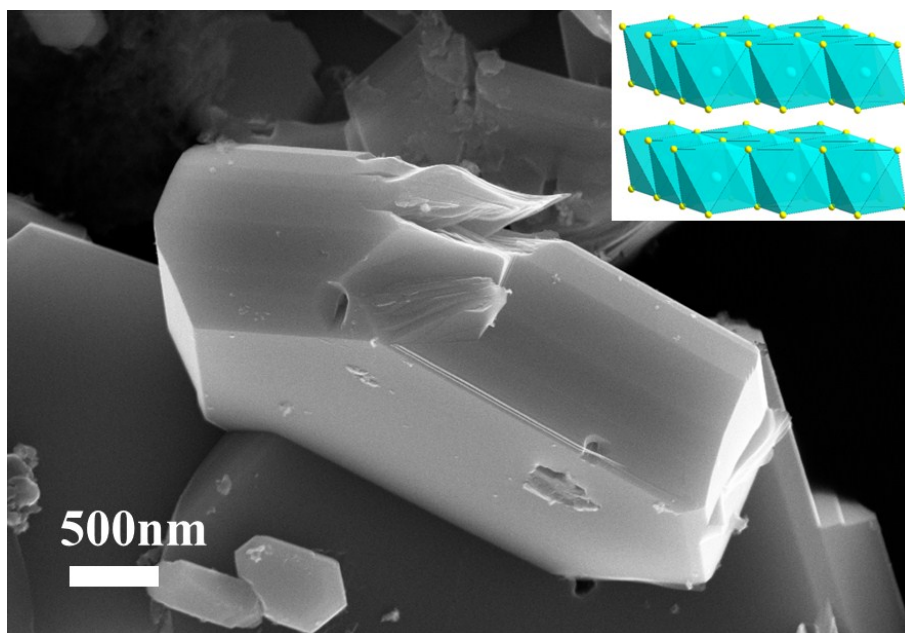


Fig. S6 SEM image of CV-TiS_{2-x} with particle size larger than 500 nm.

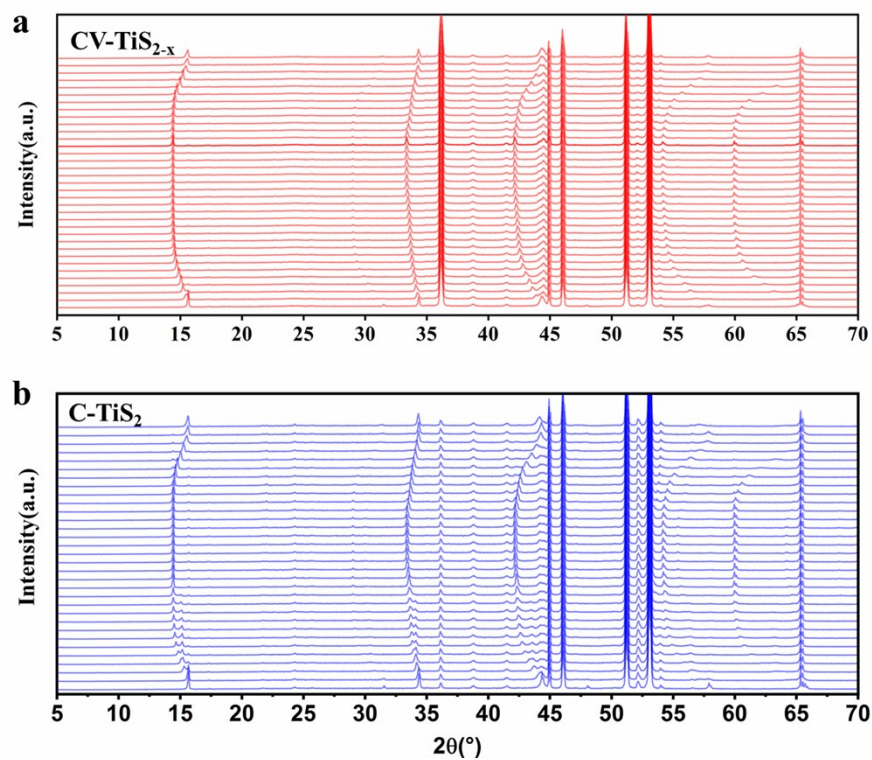


Fig. S7 In situ XRD patterns of CV-TiS_{2-x} (a) and C-TiS₂ (b) electrodes during the initial cycle at 1C.

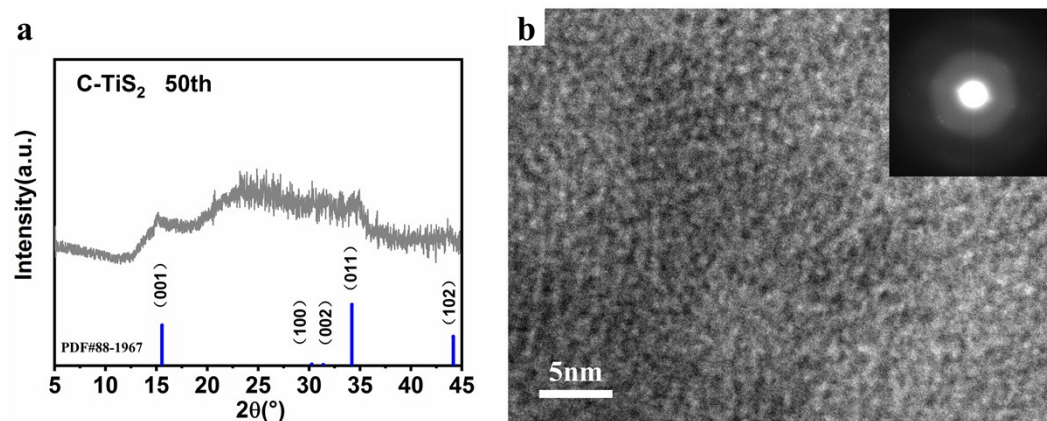


Fig. S8 XRD results of C-TiS₂ electrode after 50 cycles (a) and the corresponding TEM images (b).

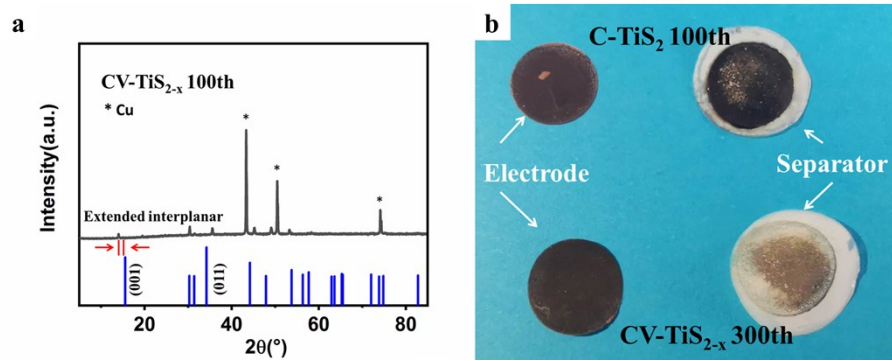


Fig. S9 XRD patterns of the CV-TiS_{2-x} after 100 cycles (a). The electrodes and separators of C-TiS₂ and CV-TiS_{2-x} batteries after cycling (b).

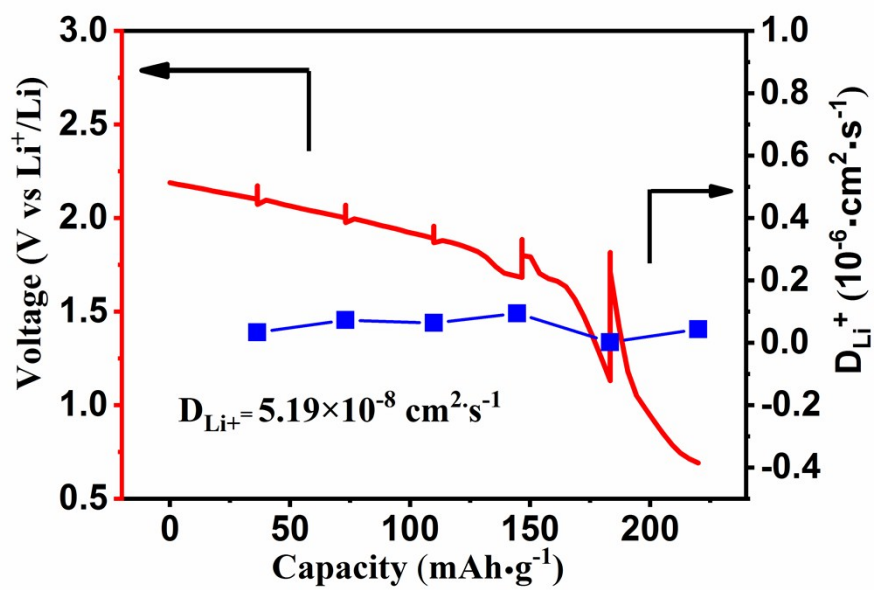


Fig. S10 GITT curves of C-TiS2 at the first cycle with a relaxation time of 2h.

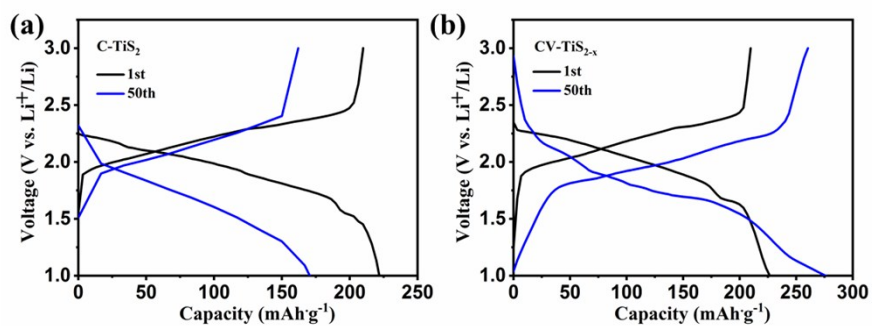


Fig. S11 Galvanostatic discharge / charge curves of CV-TiS_{2-x} (a) and C-TiS_2 (b) electrode at a current density of 1C.

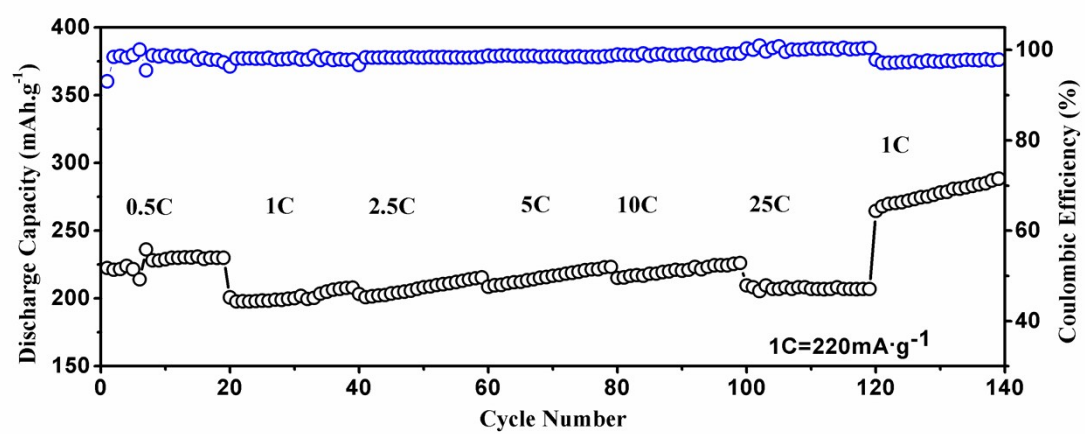


Fig. S12 The rate capability of CV-TiS_{2-x} electrode (1C=220mA·g⁻¹).

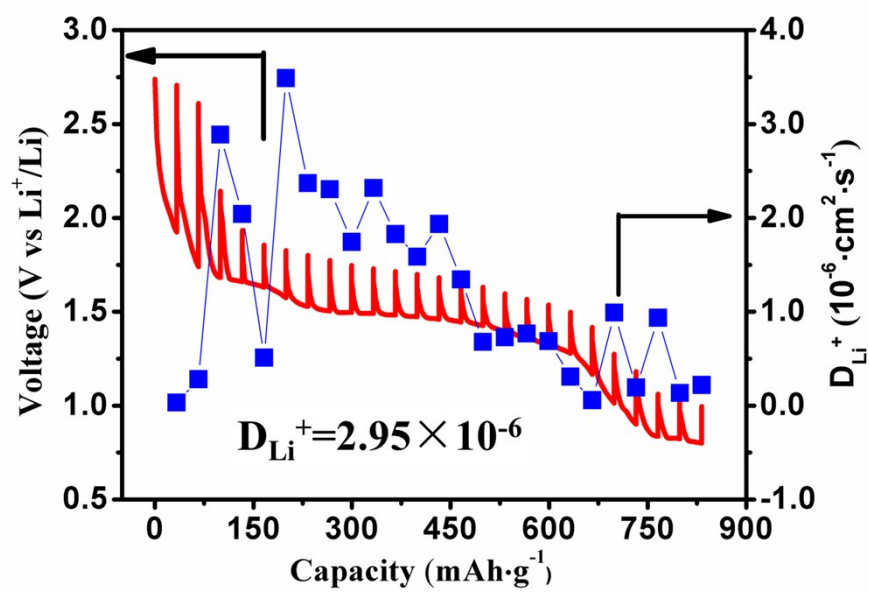


Fig. S13 GITT of CV-TiS_{2-x} electrode in the 300th discharging at 25 °C.

Table S1. The molar ratio of Ti : S in C-TiS₂ and CV-TiS_{2-x}

Samples	Ti : S molar ratio	
	based on XPS	based on ICP-OES
CV-TiS _{2-x}	1.87	1.82
C-TiS ₂	2.15	1.97

In both samples, the XPS determined stoichiometry is significantly higher than the ICP-OES determined stoichiometry. As XPS only detects the surface of the material while ICP-OES detects the bulk, this suggests that the surface of the electrode materials is more sulfur rich than the interior.

Table S2 The lattice parameters of CV-TiS_{2-x} and C-TiS₂.

	CV-TiS _{2-x}	C-TiS ₂
Lattice volume (Å ³)	56.92	56.98
Lattice-substitution	0.97	1.02
Bond length (Å)	2.412	2.423

Table S3 Electrochemical performance comparison

Chemical	Current ($\text{mA}\cdot\text{g}^{-1}$)	Capacity ($\text{mAh}\cdot\text{g}^{-1}$)	Reference
CV-TiS _{2-x}	220	650(300th)	This work
TiS _{2-x}	230	183(100th)	[3]
TiS _{2-x} nanobelt	23	224(100th)	[4]
TiS ₂	100	187(120th)	[5]

References

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