Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information

Kinetics study on intercalation pseudocapacitance of layered TiS_2 in K-ion batteries

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Experimental Section

Synthesis of Few-layered TiS_2: Sheet-like TiS_2 powder was purchased from Sigma-Aldrich. The few-layered TiS_2 was synthesized by Li intercalation method. Briefly, Sheet-like TiS_2 materials, Super P and PVDF were mixed in a mole ratio of 8: 1: 1 with N-methyl pyrrolidone (NMP) solvent. The slurry was coated on a Cu foil with thickness of 60 μm via a MSK-AFA-I coating machine (Hefei Kejing Materials Technology Co.,Ltd). After dried in vacuum oven at 120 ^oC for 12 h, the electrode was punched into Φ = 1.2 cm disks. The loading mass of TiS_2 is 1.7 ± 0.1 mg cm^{-2}. The cell was discharged to 1.5 V at 20 mA g^{-1}, and the electrode was washed with diethyl carbonate (DEC) for 2 times. After that, the washed electrode was put in deionized water, sealed in a container and ultrasonic treated. The exfoliated TiS_2 was washed by deionized water for 3 times and then freeze dried. The final few-layered TiS_2 product was then obtained.

Materials Characterization: Powder X-ray diffraction (XRD) measurement was performed on a Bruker D8 Focus Powder X-ray diffractometer using Cu *Kα* radiation (40 kV, 40 mA). Field-emission scanning electron microscopy (FE-SEM) was performed on a field emission Hitachi S-4800 instrument, operating at an accelerating voltage of 10 kV. Transmission electron microscope (TEM) was performed using a FEI Tecnai G_2S-Twin instrument with a field emission gun operating at 200 kV. Atomic force microscopy (AFM) observation was carried out with an AFM system (Dimension Icon, Bruker).

Electrochemical Measurement: The electrochemical performance of TiS_2 material for K^+ (de)-intercalation was evaluated by galvanostatic charge/discharge technique. To prepare working electrode, TiS_2, Super P and PVDF were mixed in a mole ratio of 8: 1: 1 with N-methyl pyrrolidone (NMP) solvent. The slurry was coated on a Cu foil with thickness of 60 μm via a MSK-AFA-I coating machine (Hefei Kejing Materials Technology Co.,Ltd). After dried at 120 ^oC for 12 h, the electrode was pressed at 20 M Pa and then punched into disks (Φ = 1.2 cm). The loading mass of TiS_2 is 1.7 ± 0.1 mg

cm^{-2}. 2025 coin-type cells were assembled in an argon-filled glove box, together with a piece of metal potassium disk as counter electrode and glass fiber (GF/C, Whatman) as separator, respectively. The electrolyte was 0.8 M KPF_6 in a mixture of ethylene carbonate (EC) and DEC (1:1, w/w). Galvanostatic charge-discharge cycling tests were performed in a voltage range of 0.4-3.0 V at different current rates on a Land CT2001A battery testing system (Land, P. R. China) at room temperature. In addition, GITT, PITT and CV measurements were performed on a VMP3 electrochemical workstation (Bio-Logic, France). For each GITT step, the battery was discharged/discharged with a current flux of 10 mA g^{-1} for 30 min, followed by an open circuit stand for 4 h to reach the quasi-equilibrium state. For PITT test, the battery was applied with a constant voltage V_0 and this could generated a current as a function of time. The step is ended when the current is below 0.01 C (1C = 170 mA g^{-1}). Then the battery is applied with another voltage of V_0-ΔE, and then V_0-2ΔE…V_0-nΔE, where ΔE is 10 mV in this work.

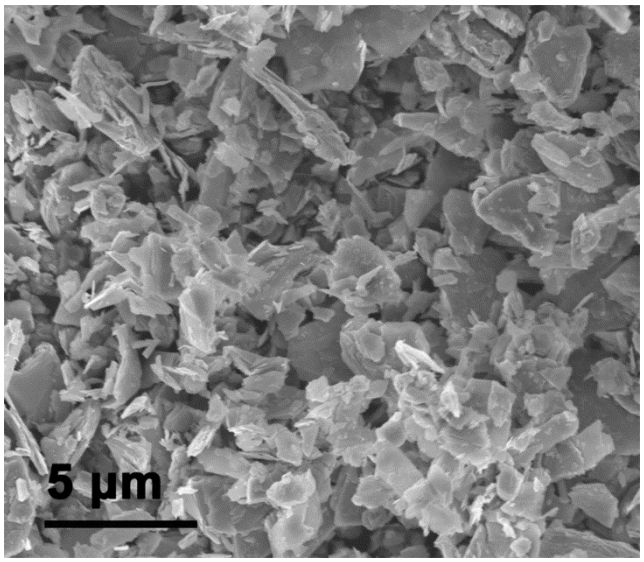

Fig. S1 SEM image of sheet-like TiS_2 powder.

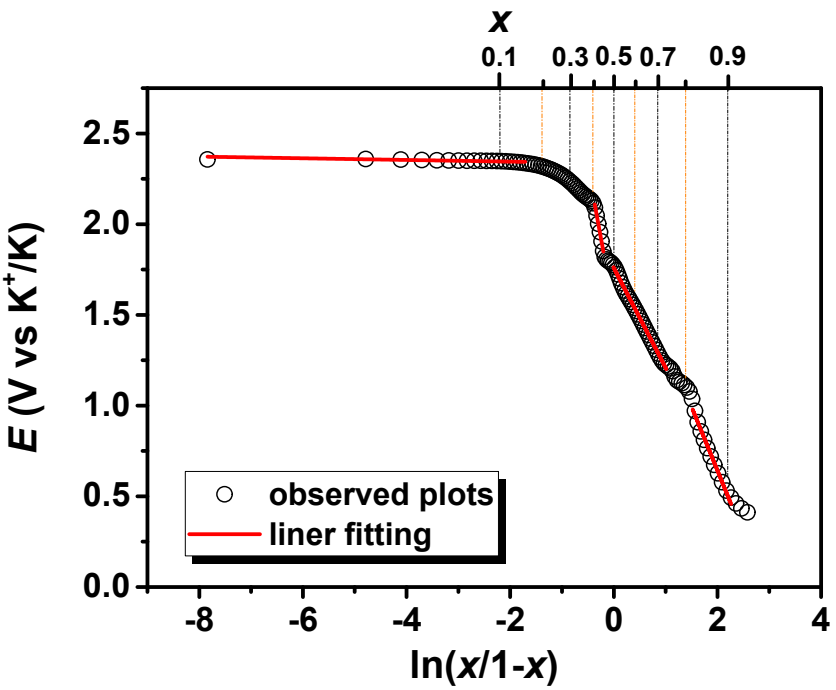

Fig. S2 Relation of E as a function of ln(x/1-x).

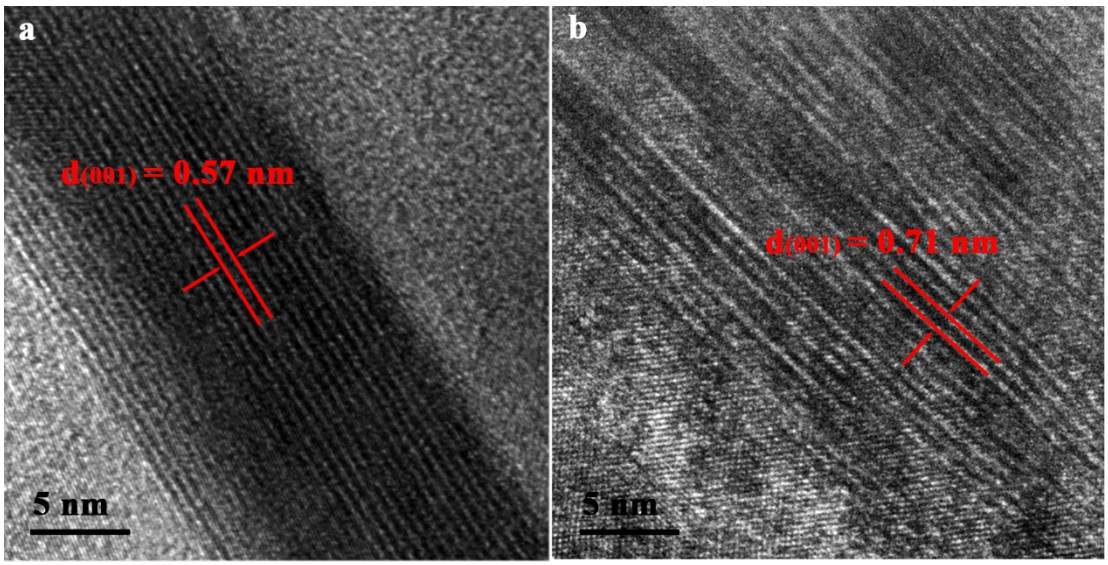

Fig. S3 HRTEM images of (a) origin TiS_2 and (b) TiS_2 discharged to 0.4 V.

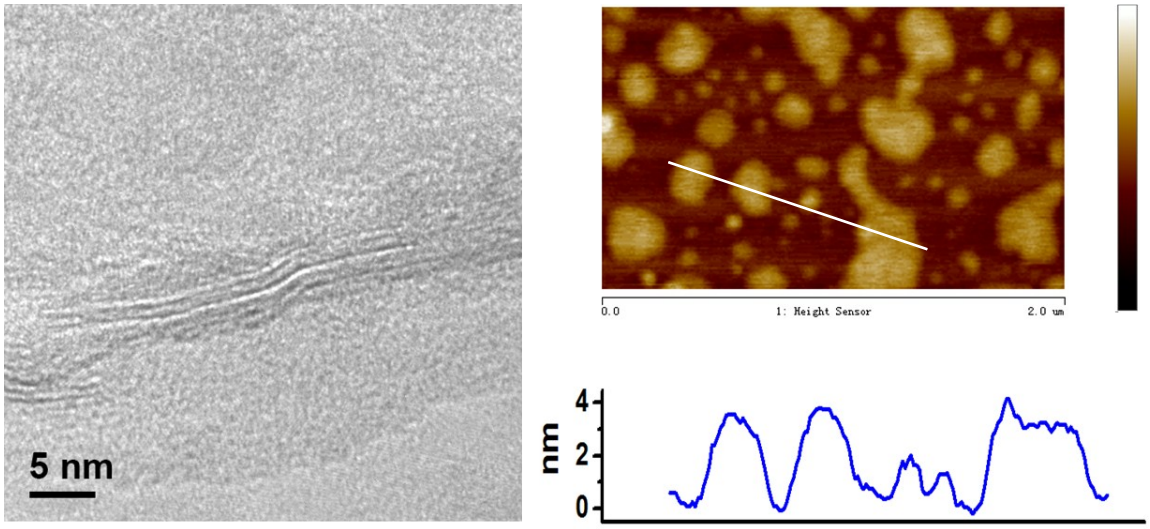

Fig. S4 HRTEM image and AFM image of exfoliated few-layered TiS_2.

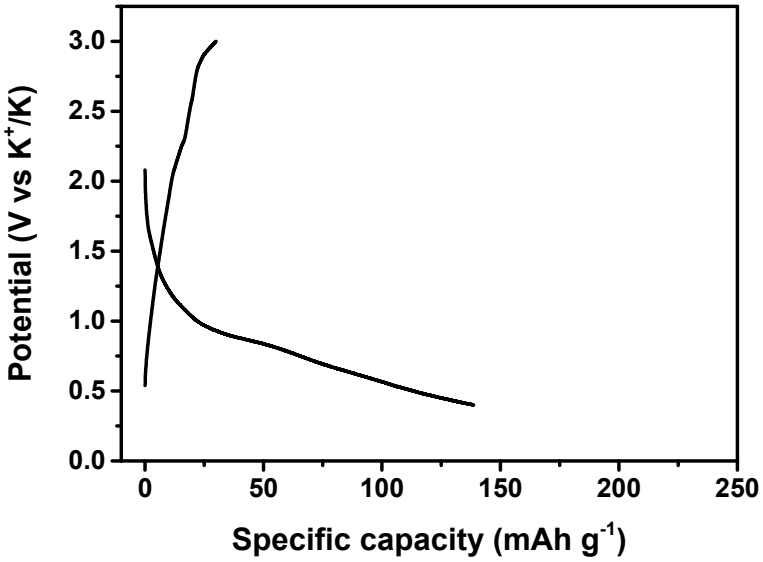

Fig. S5 Discharge/charge profiles of exfoliated few-layer TiS_2 at current density of 20 mA g^{-1}.

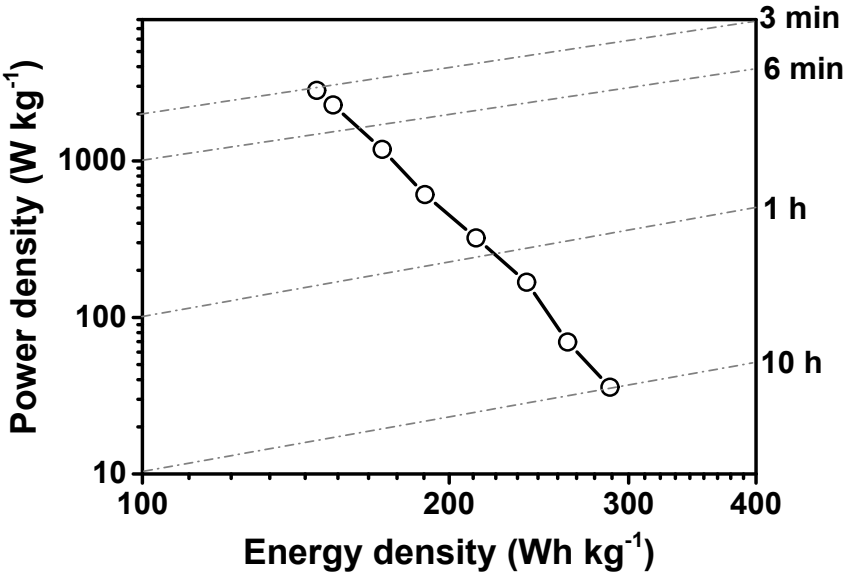

Fig. S6 Ragone plots of TiS_2 based on mass of cathode materials.

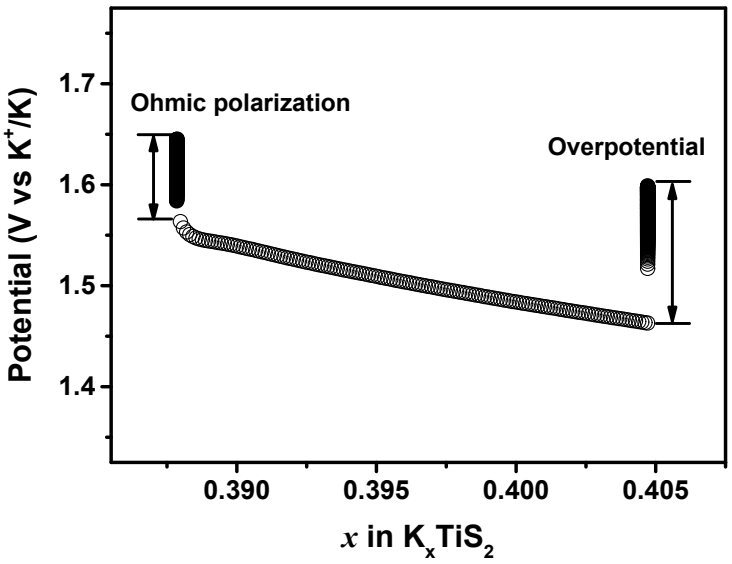

Fig. S7 Typical titration step of TiS_2 at $x = 0.388$.

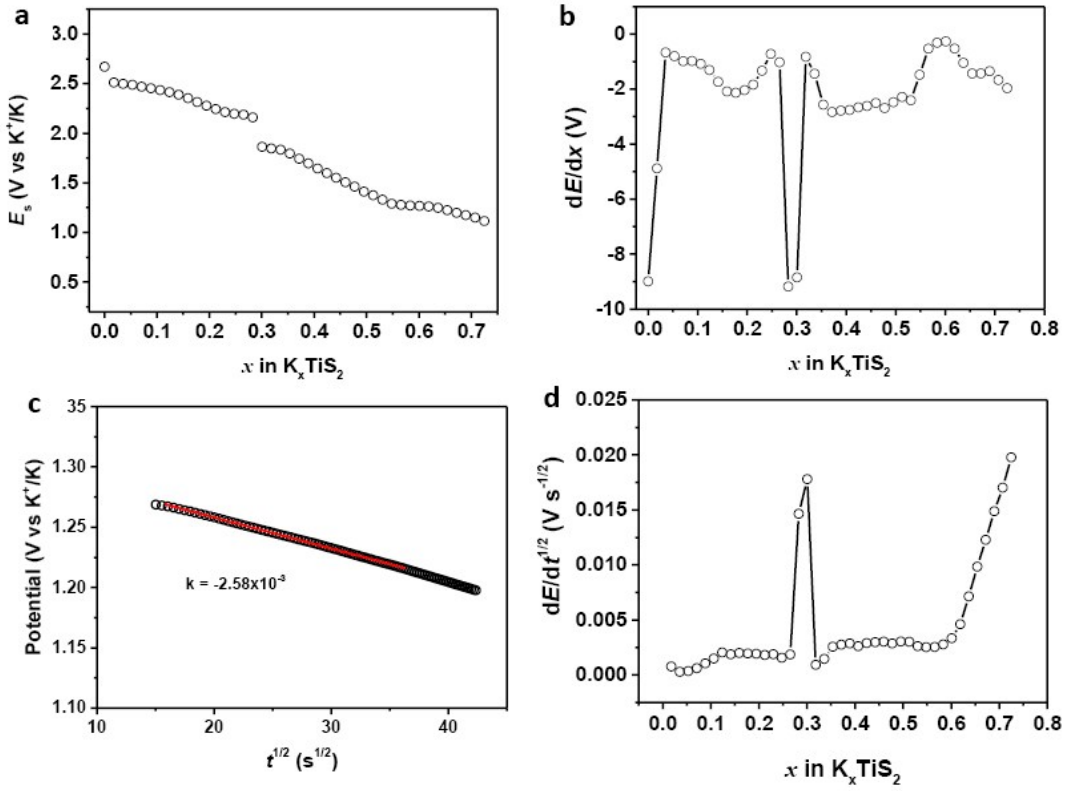

Fig. S8 (a) E_s versus x curves of TiS_2, (b) dE_s/dx values of TiS_2. (c) Typical E versus $t^{1/2}$ plot of TiS_2 and (d) dE/d$t^{1/2}$ values of TiS_2.

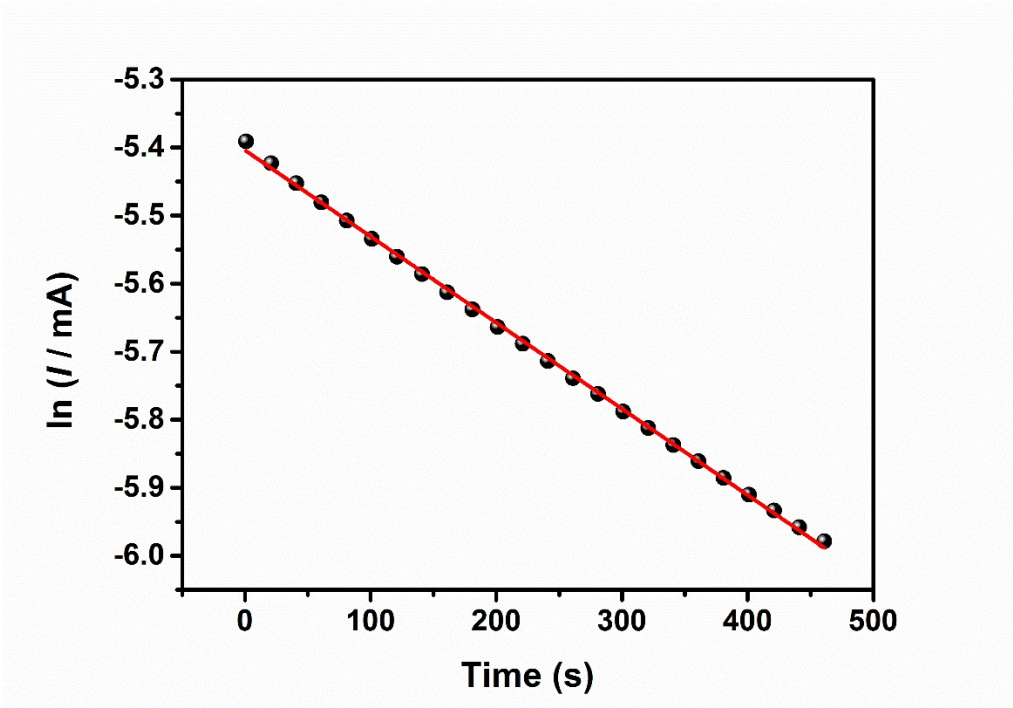

Fig. S9 A typical current response of TiS_2 under potential step from 2.25 V to 2.24 V.

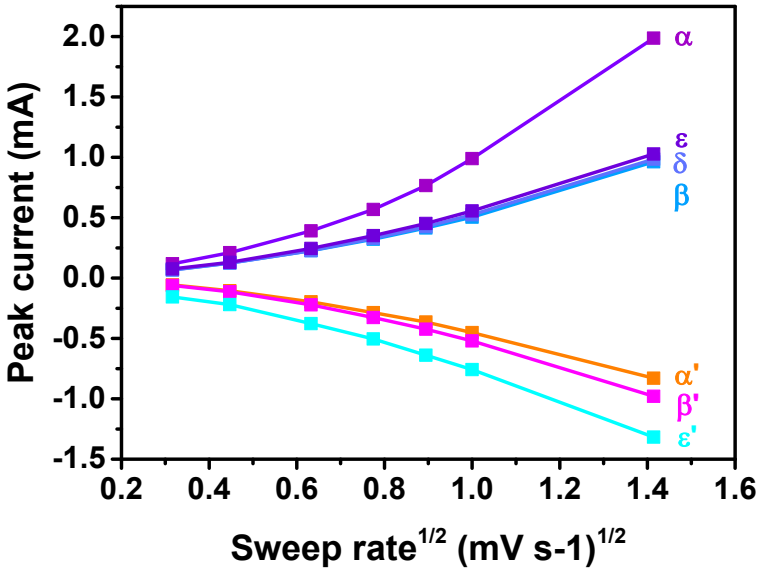

Fig. S10 Relationship between peak current and square root of sweep rate.