Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

V_2CT_X Catalyzes Polysulfide Conversion to Enhance Redox Kinetics of Li−S Batteries

Fengfeng Han, Qi Jin, Junpeng Xiao, Lili Wu*, Xitian Zhang*

Key Laboratory for Photonic and Electronic Bandgap Materials, Ministry of Education, School of Physics and Electronic Engineering, Harbin Normal University, Harbin 150025, people's Republic of China.

* Corresponding author: wll790107@hotmail.com; xtzhangzhang@hotmail.com

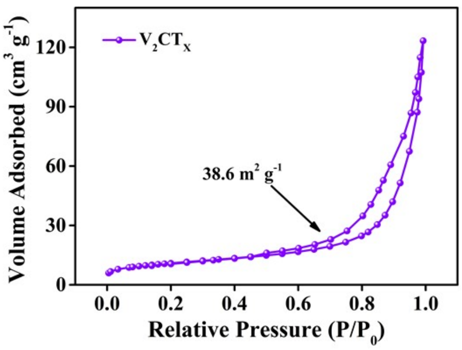

Fig. S1. Nitrogen adsorption/desorption isotherm curve of V_2CT_X nanobelts.

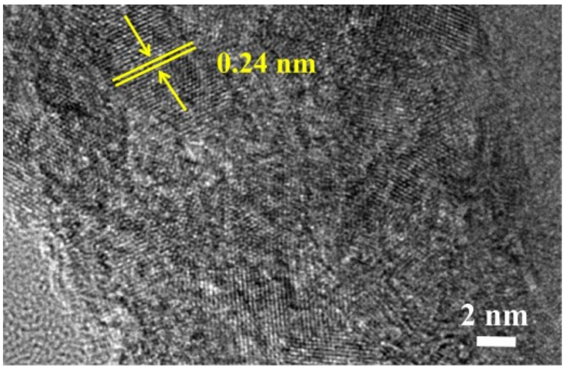

Fig. S2. HRTEM image of a V_2CT_X nanobelt.

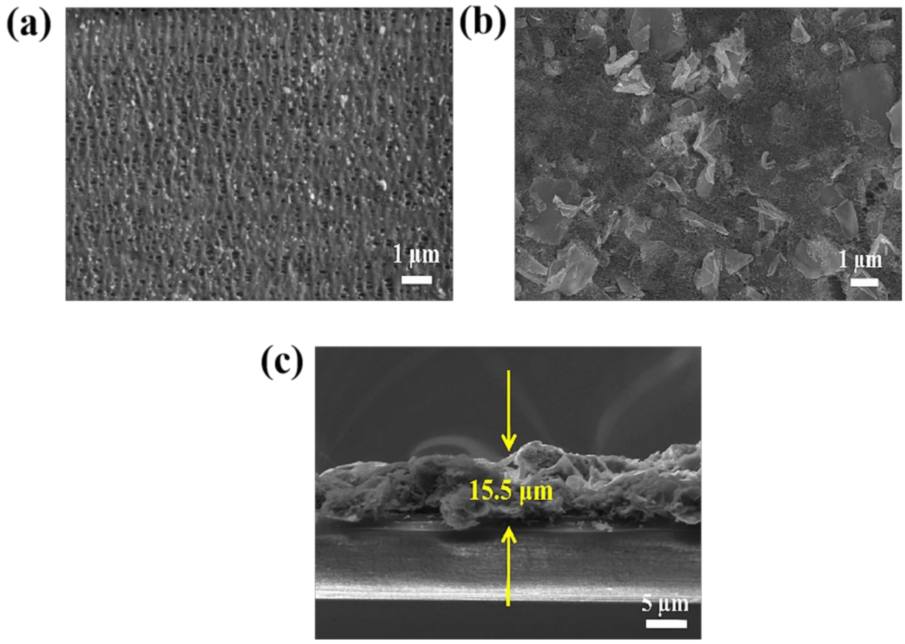

Fig. S3. SEM images of (a) PP and (b) KB/V_2CT_X-PP separators. (c) Cross-sectional SEM image of KB/V_2CT_X interlayer.

Fig. S4. Digital photographs of Li_2S_6 solution and after the addition of KB/V_2CT_X.

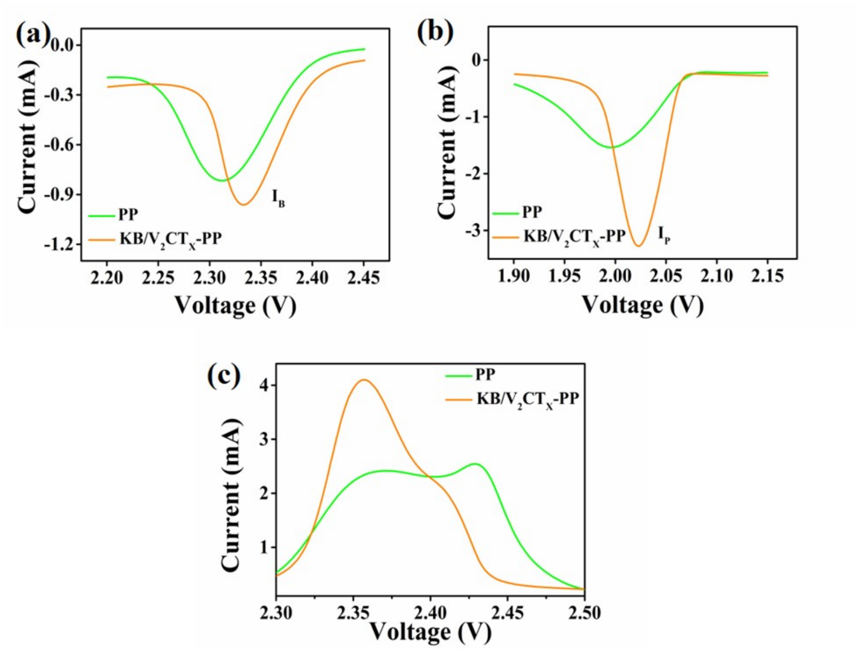

Fig. S5. (a, b) Magnified cathodic peaks and (c) anode peaks of the two cells.

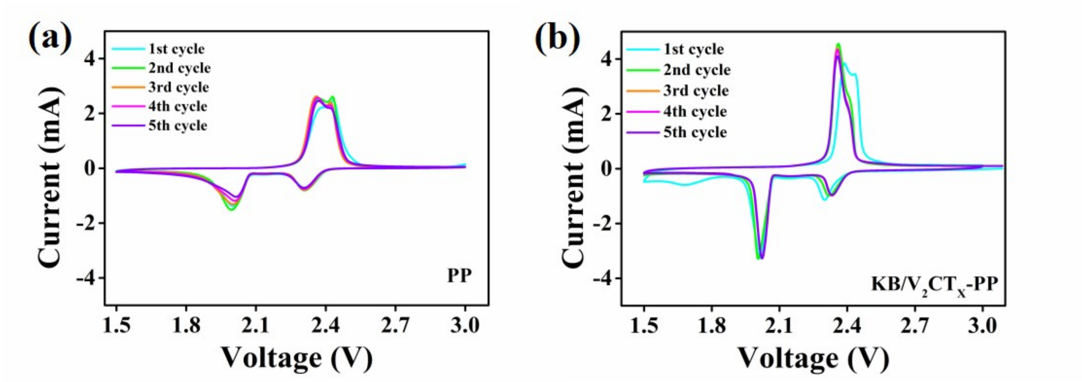

Fig. S6. CV profiles of (a) PP and (b) KB/V_2CT_X-PP cells for consecutive cycles.

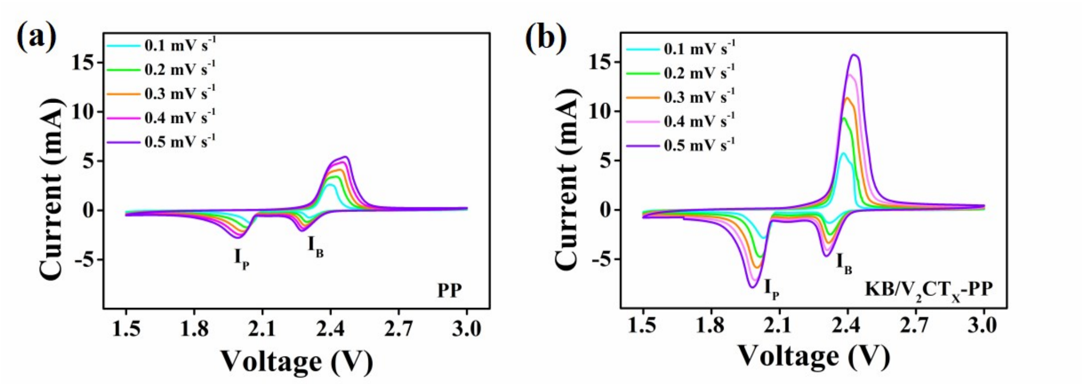

Fig. S7. CV curves of (a) PP and (b) KB/V_2CT_X-PP cells at different scan rates.

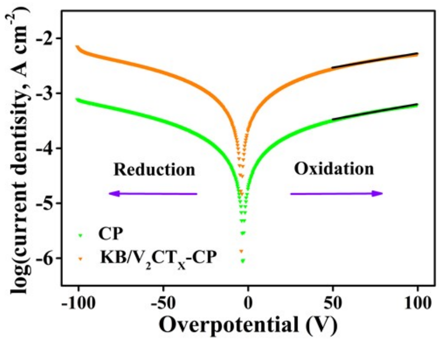

Fig. S8. LSV analyses of KB/V_2CT_X-CP and CP cells with Li_2S_6 catholyte.

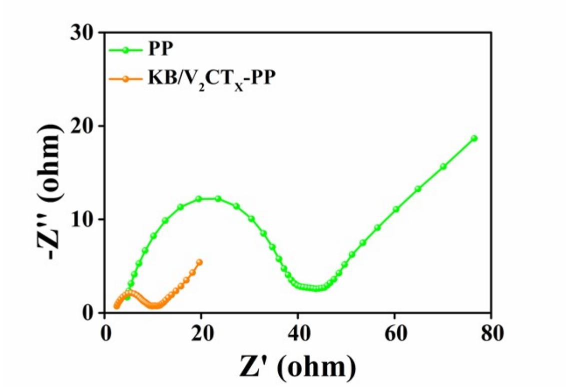

Fig. S9. EIS curves of PP and KB/V_2CT_X-PP cells.

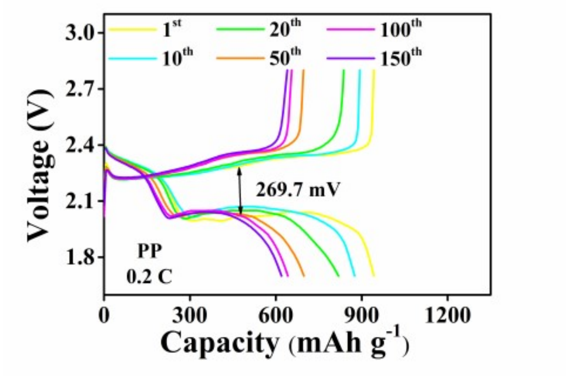

Fig. S10. GCD curves of PP cells at 0.2 C.

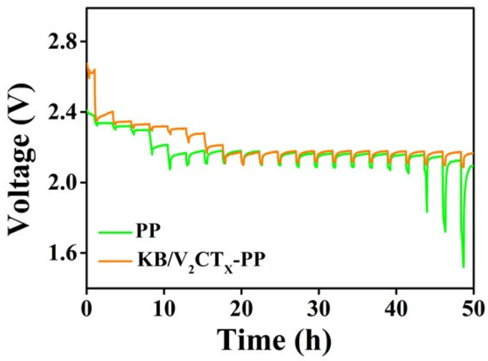

Fig. S11. GITT curves of cathodes with PP and KB/V_2CTx-PP separators during discharge process.

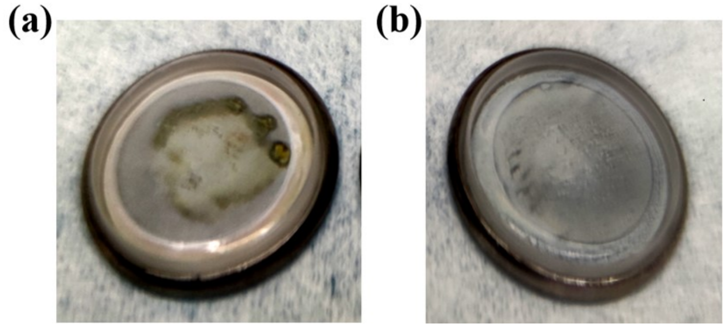

Fig. S12. Photographs for (a) PP and (b) KB/V_2CT_X-PP separators toward Li metal anode after 150 cycles at 0.2 C.

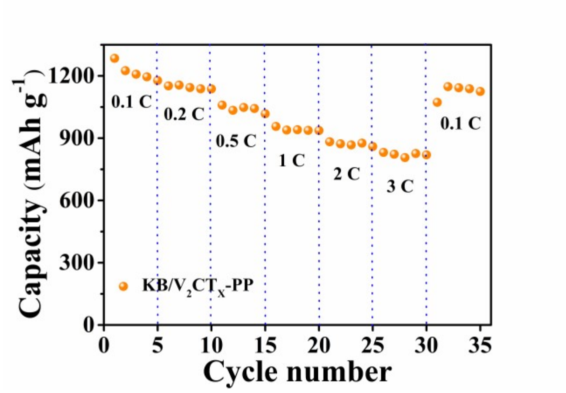

Fig. S13. Rate performance of KB/V_2CT_X-PP cells (1 C = 1675 mA g^{-1})

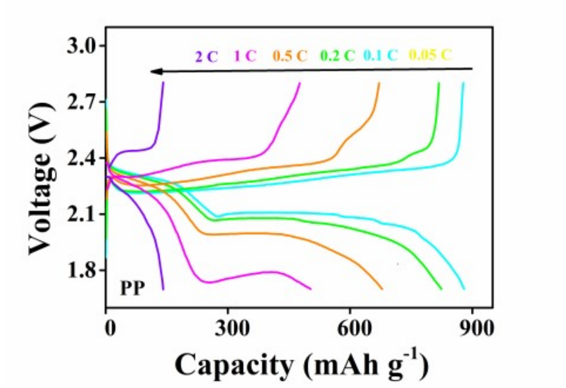

Fig. S14. GCD curves of a PP cells at different rates.

Table S1. Comparison of the cycle performance between this work and other previously reported similar materials

Materials	S loading (mg cm^{-2})	Rate (C)	Initial capacity (mAh g^{-1})	Cycle Number	Capacity decay (% per cycle)	Ref.
d-Ti_3C_2	0.7-1	0.5	899	50	0.64	[1]
$Ti_3C_2T_x$ aerogel	1.2	1	980	1500	0.037	[2]
CNTs/$Ti_3C_2T_x$	0.8	1	987	600	0.063	[3]
$Ti_3C_2T_x$@Nafion	2	1	920	1000	0.03	[4]
Nb_2O_5-CNT	1.3-1.5	0.2	1286	100	0.23	[5]
S@V_2C-Li/C	3.0	0.1	1140	100	0.096	[6]
V_2C/V_2O_5/CNTs	2.0	1	1055.2	500	0.034	[7]
KB/V_2CT_X	1.2	1	1069	1000	0.049	This work

Note 1. The detail calculation scheme of relative activation energy.

CV tests were performed under a scan rate (0.1 mV s^{-1}) at 298 K as shown in Figure 2a.

Correspondingly, the relationship between electrode potential and activation energy over the Catalyzed-free and In-based batteries could be calculated according to the equation (1):

$$E_a = E_a^0 + \alpha zF\varphi_{cathode}(Ox|Red)_{IR} \quad (1)$$

where E_a is the activation energy of reduction process, E_{a0} is the intrinsic activation energy, α is the symmetry coefficient, z is the number of charge transfer, F is the Faraday's constant, $\varphi_{cathode}(Ox|Red)_{IR}$ is the irreversible potential during cycling.

The Tafel curve calculation formula (2):

$$\eta_{cathode} = \frac{RT}{\alpha zF}\ln j_0 - \frac{RT}{\alpha zF}\ln j_{cathode} \quad (2)$$

where $\eta_{cathode}$ is the overpotential of the cathode, j_0 is the exchange current density, $j_{cathode}$ is the current of the cathode. The equation can be written in a more concise form:

$$\eta_{cathode} = a + b\ln j_{cathode} \quad (3)$$

$$b = -\frac{RT}{\alpha zF} \quad (4)$$

where a is the intercept of Tafel curve, b is the slop of Tafel curve. Therefore, the equation (1) can be written in a more concise form:

$$E_a = E_a^0 - \frac{RT}{b}\varphi_{cathode}(Ox|Red)_{IR} \quad (5)$$

Based on the intercept and slop of the Tafel curve as shown in Figure. 3b, c the activation energy during the discharge and charge process can be calculated.

The activation energy corresponding to the reduction of S_8 to the long-chain Li_2S_n:

PP cells: $Ea_1 = Ea_1^0 – 115.77$ kJ mol^{-1}

KB/V_2CT_X-PPcells: $Ea_1' = Ea_1^0 – 144.4$ kJ mol^{-1}

The difference in activation energy could be calculated by subtracting the activation energy of In-free electrode from that of In-based electrode.

Ea_1'- Ea_1 = (Ea_1^0–144.4) kJ mol-1– (Ea_1^0–115.77) kJ mol^{-1}= -28.63 kJ mol^{-1}

The activation energy of long-chain Li_2S_n to Li_2S:

PP cells: $Ea_2 = Ea_2^0 – 112.32$ kJ mol^{-1}

KB/V_2CT_X-PP cells: Ea2’ = Ea_2^0–137.14 kJ mol^{-1}

Ea_2'- Ea_2 = (Ea_2^0–137.14) kJ mol^{-1}– (Ea_2^0–112.32) k J mol^{-1}= -24.82 kJ mol^{-1}

References

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