

Supporting Information:

Vanadium Based Carbide-Oxide Heterogeneous V₂O₅@V₂C Nanotube Array for High-Rate and Long-Life Lithium-Sulfur Batteries

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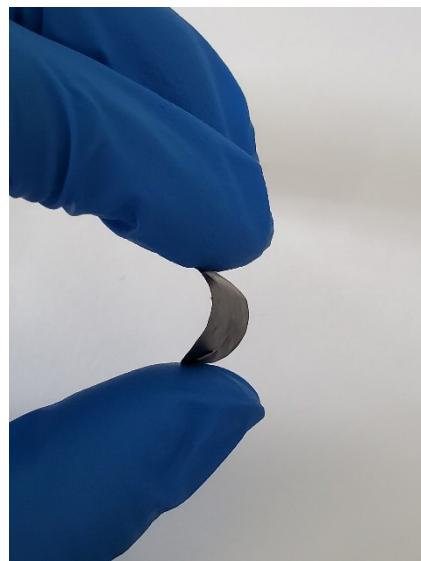


Figure S1 The $\text{V}_2\text{O}_5@\text{V}_2\text{C}/\text{S}$ cathode.

The amount of pole piece prepared for $8.4 \text{ mg}\cdot\text{cm}^{-2}$: 1.68 g sublimed sulfur, 0.42 g $\text{V}_2\text{O}_5@\text{V}_2\text{C}$, and the coating thickness is about 70 microns; the amount of pole piece prepared for $4.2 \text{ mg}\cdot\text{cm}^{-2}$: 0.84 g sublimed sulfur, 0.21 g $\text{V}_2\text{O}_5@\text{V}_2\text{C}$, the coating thickness is about 45 microns; the amount of pole piece prepared for $2.0 \text{ mg}\cdot\text{cm}^{-2}$: 0.40g sulfur, 0.10 g $\text{V}_2\text{O}_5@\text{V}_2\text{C}$, the coating thickness is about 25 microns; during the battery preparation and assembly process, the size of the aluminum foil is $200 \text{ mm}\times100 \text{ mm}$, use a microtome to cut the positive pole piece with a diameter of 15 mm, the electrolyte dosage is 80-120 microliters, the diameter of the cut diaphragm disc is 16 mm, the thickness of the metal lithium sheet used is 0.6 mm, and the diameter is also 15 mm.



Figure S2 Digital photo of removable three-electrode battery.

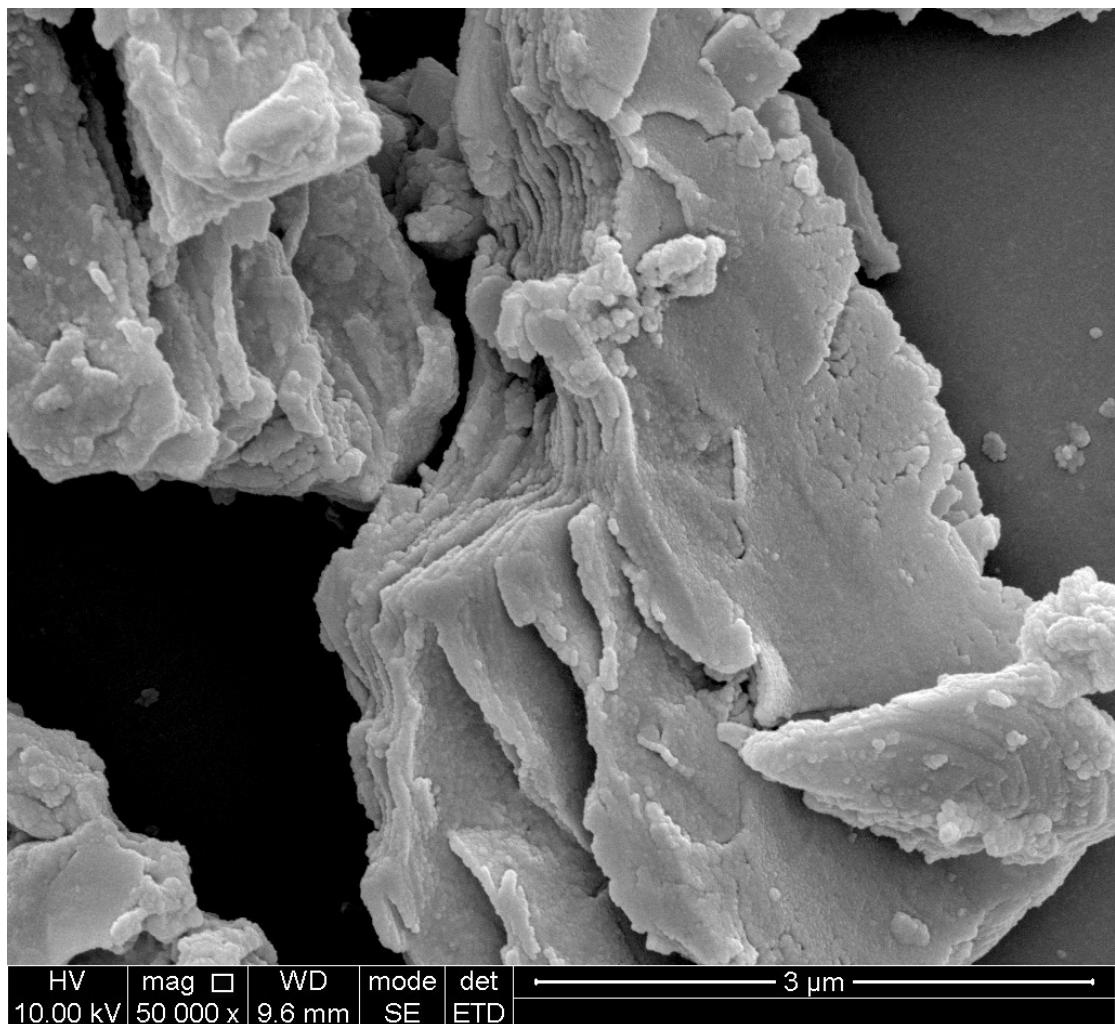


Figure S3 SEM graph of V₂C-MXene after hydro-thermal treatment.

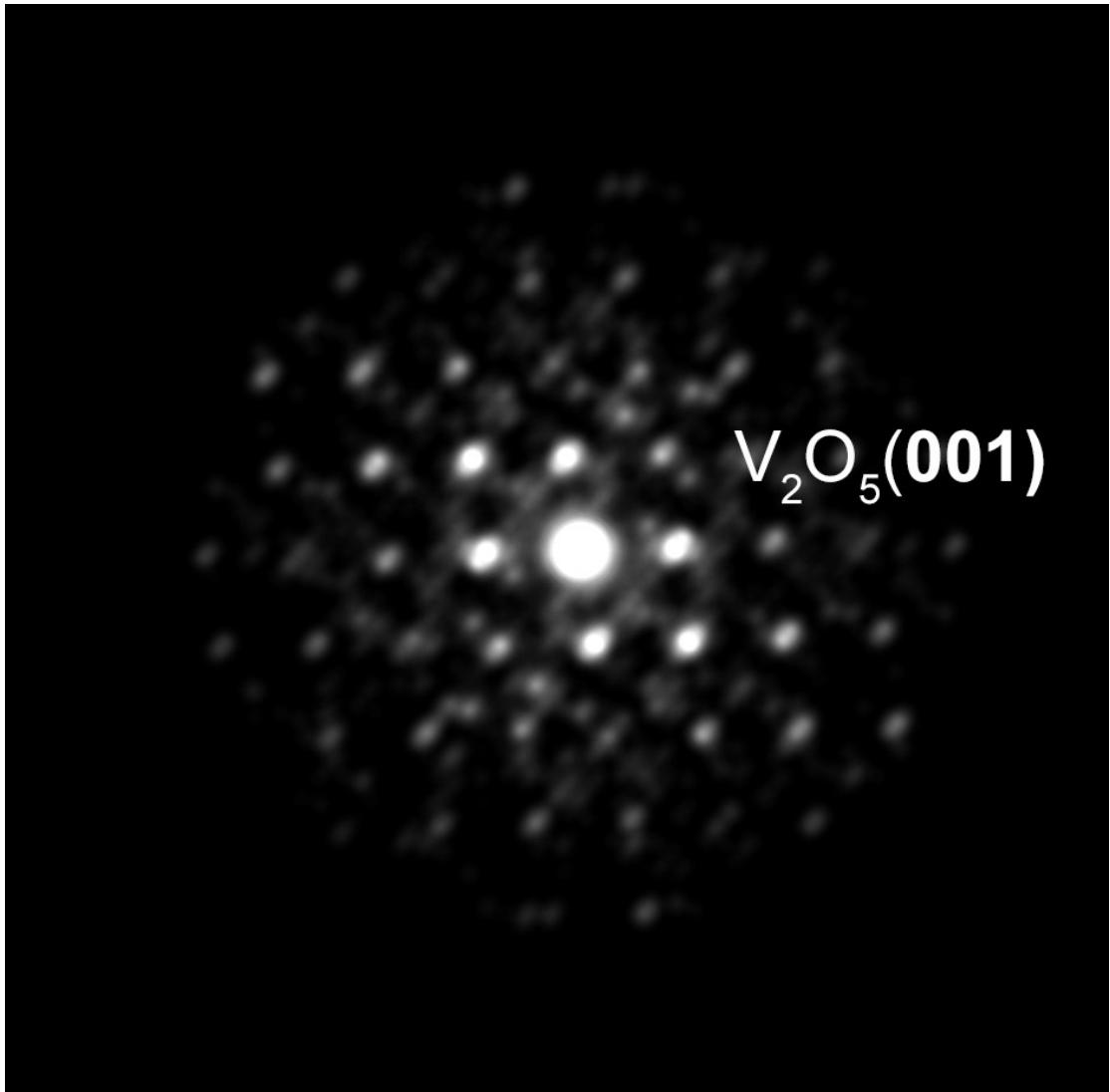


Figure S4 The selected electron diffraction FFT diagram.

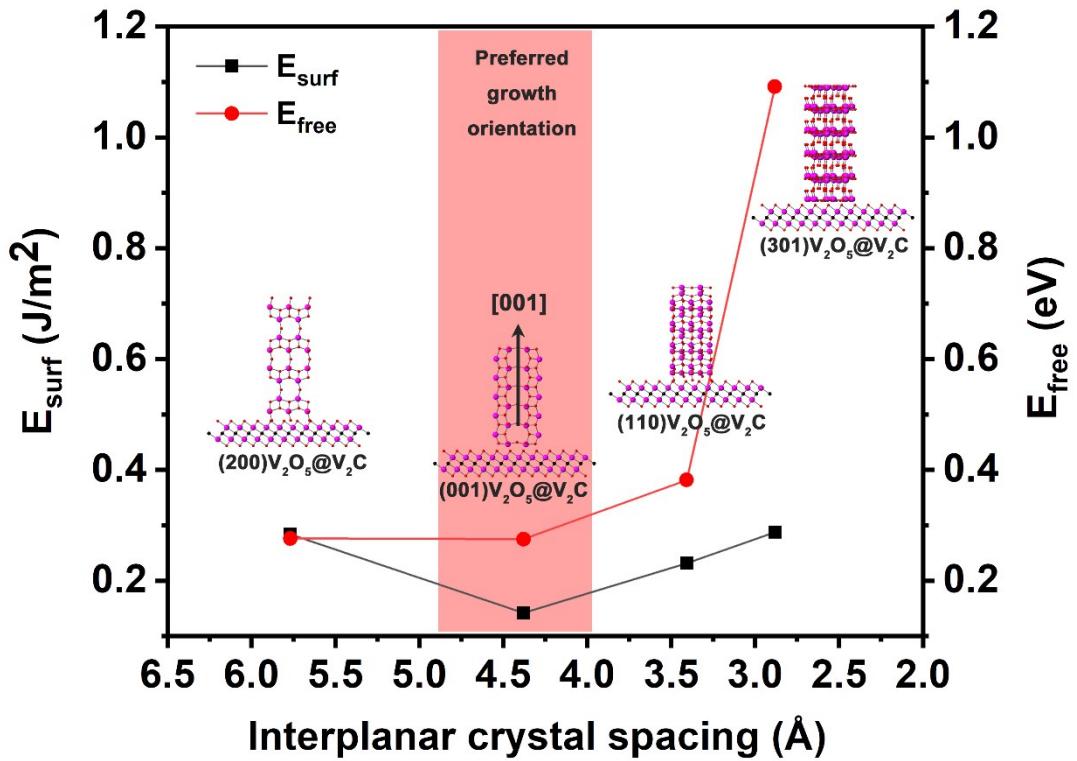


Figure S5 Surface energy and interface free energy calculation for V₂O₅@V₂C.

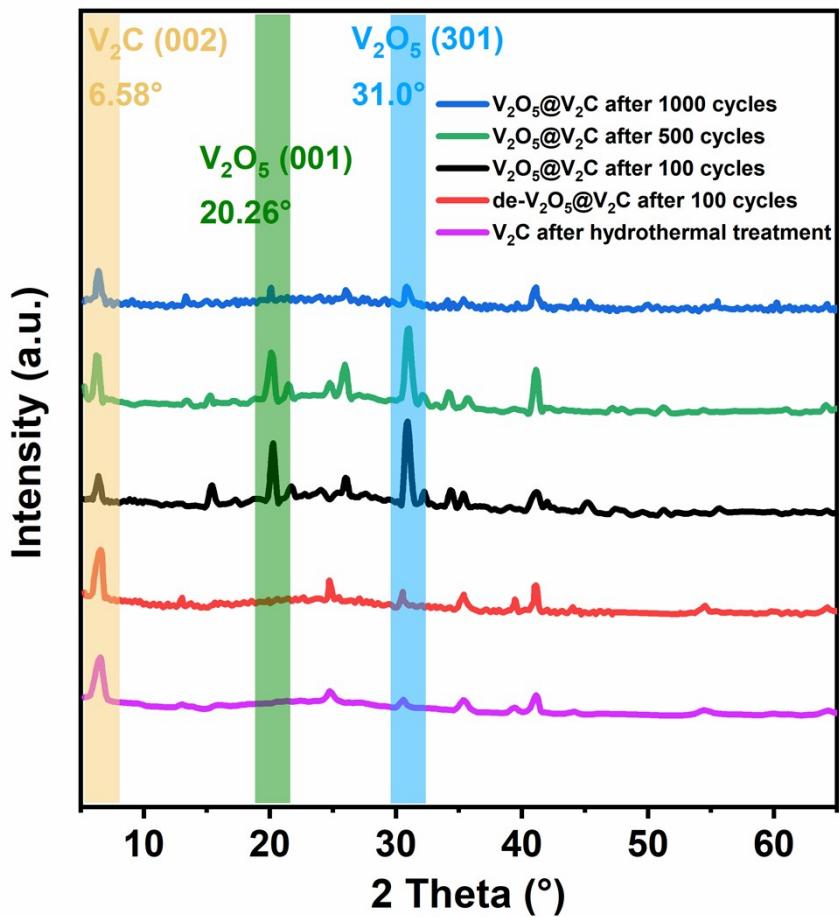


Figure S6 The XRD spectrum of V₂C, V₂O₅@V₂C after different cycles and de-V₂O₅@V₂C.

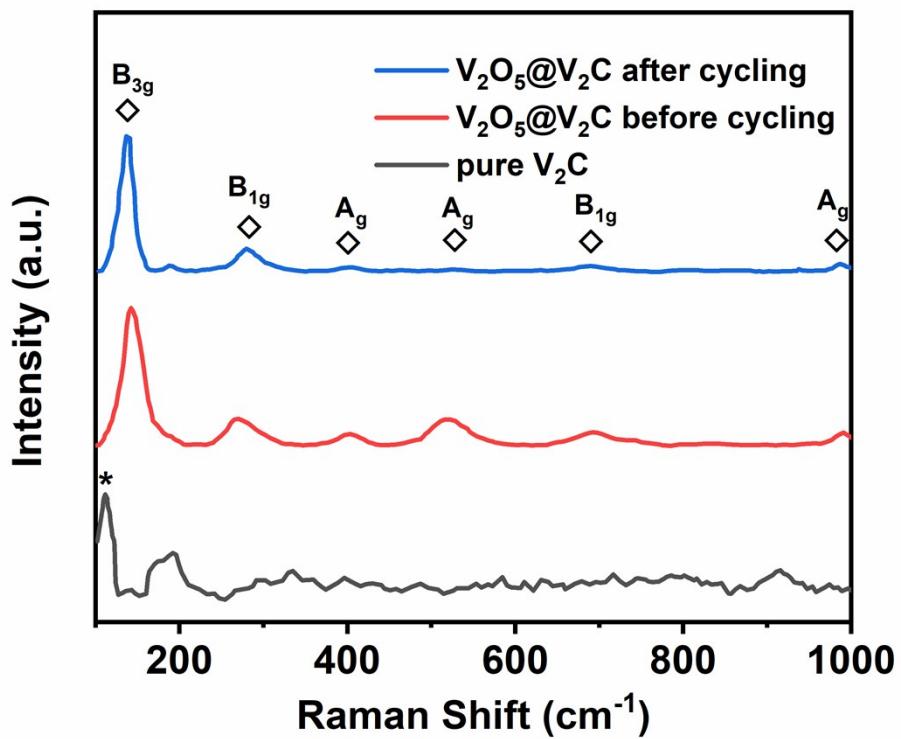


Figure S7 The Ranman spectrum of $\text{V}_2\text{O}_5@\text{V}_2\text{C}$ after & before cycling and pure V_2C .

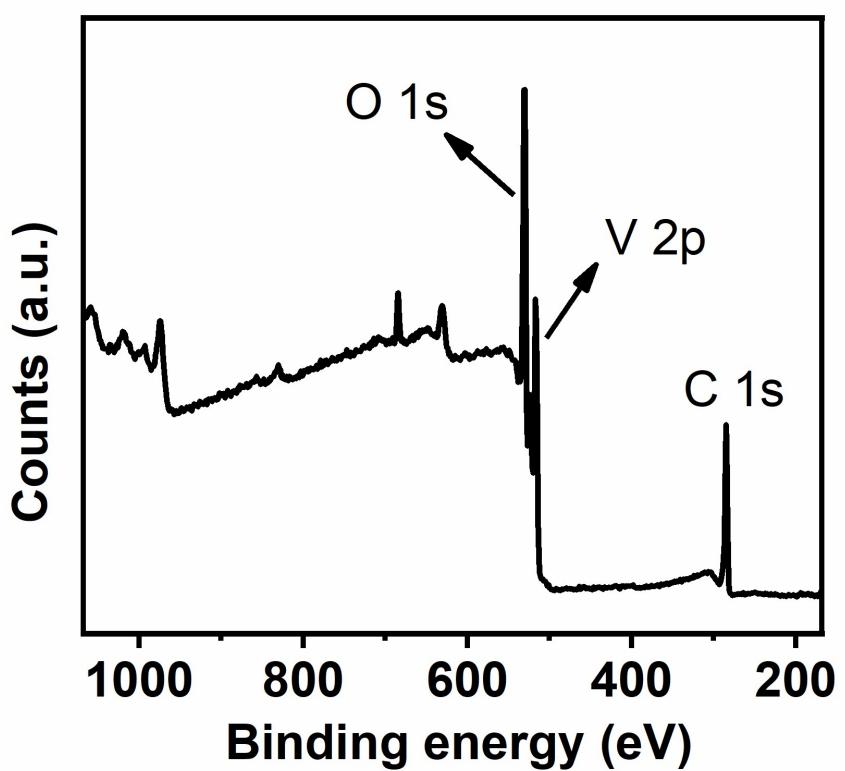


Figure S8 XPS full spectrum of $\text{V}_2\text{O}_5@\text{V}_2\text{C}$.

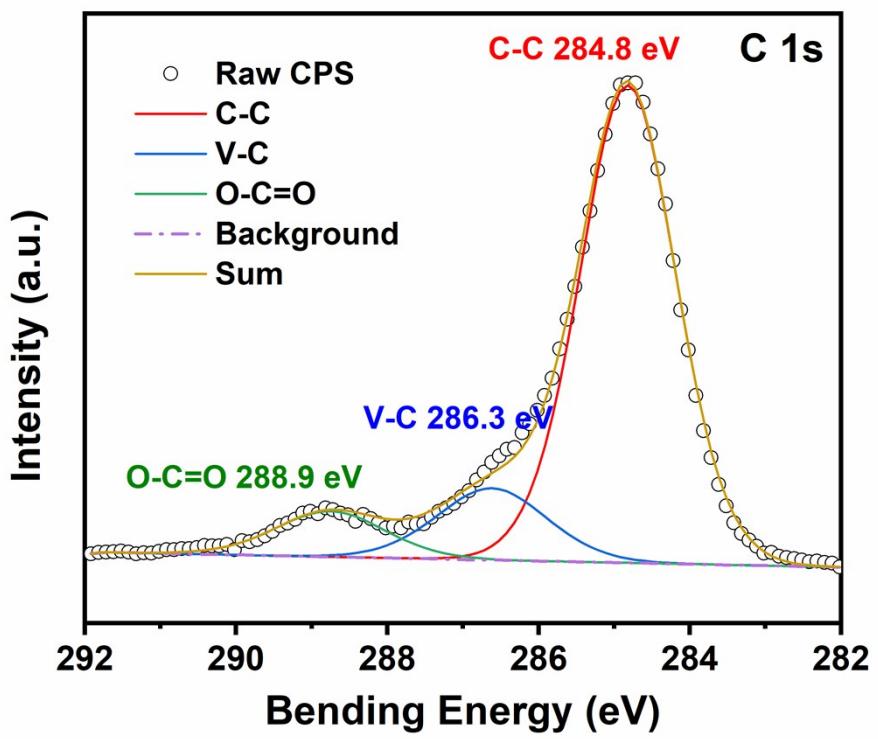


Figure S9 The XPS spectrum of C1s.

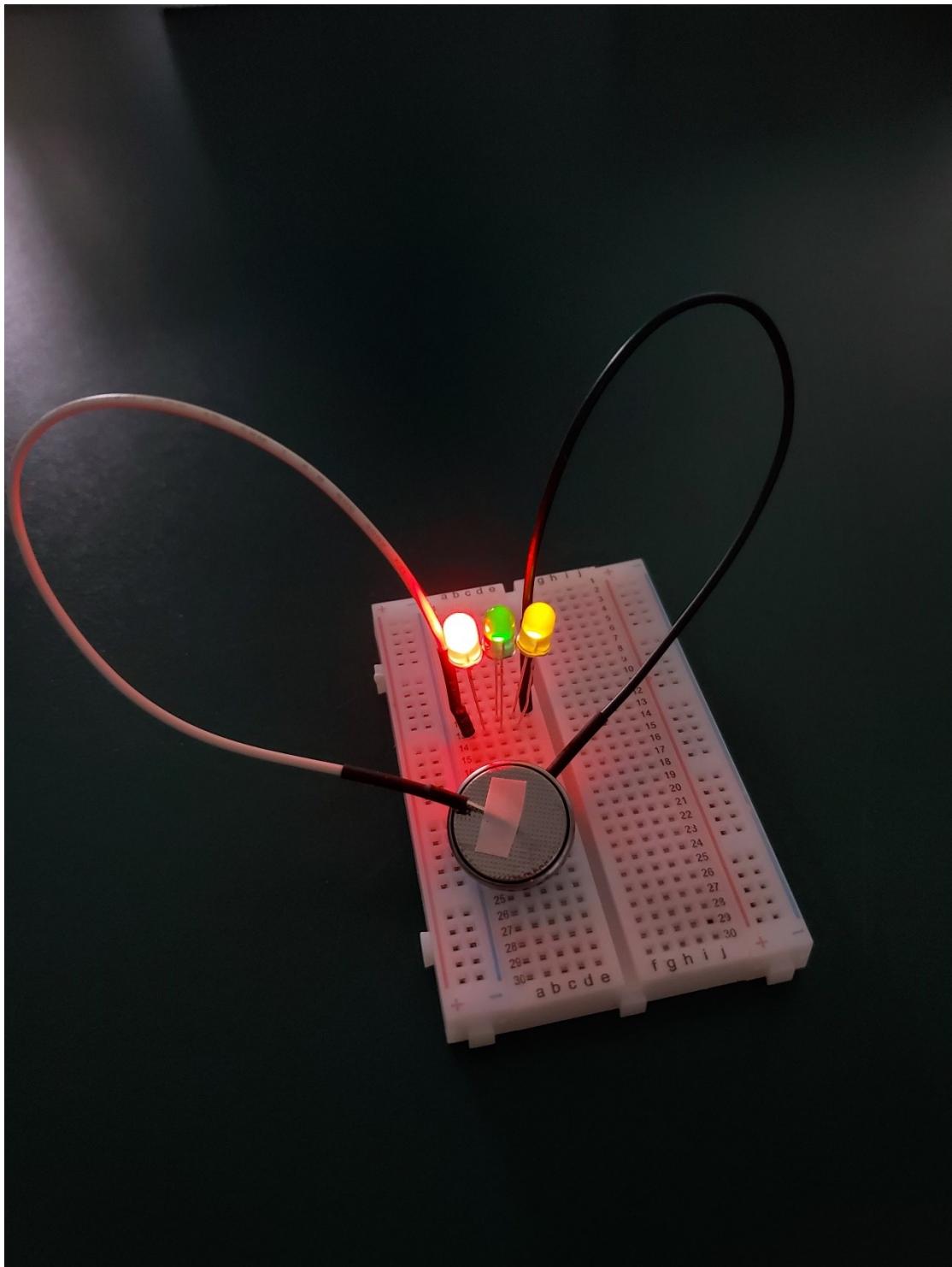


Figure S10 The actual working diagram of as-assembled lithium sulfur battery.

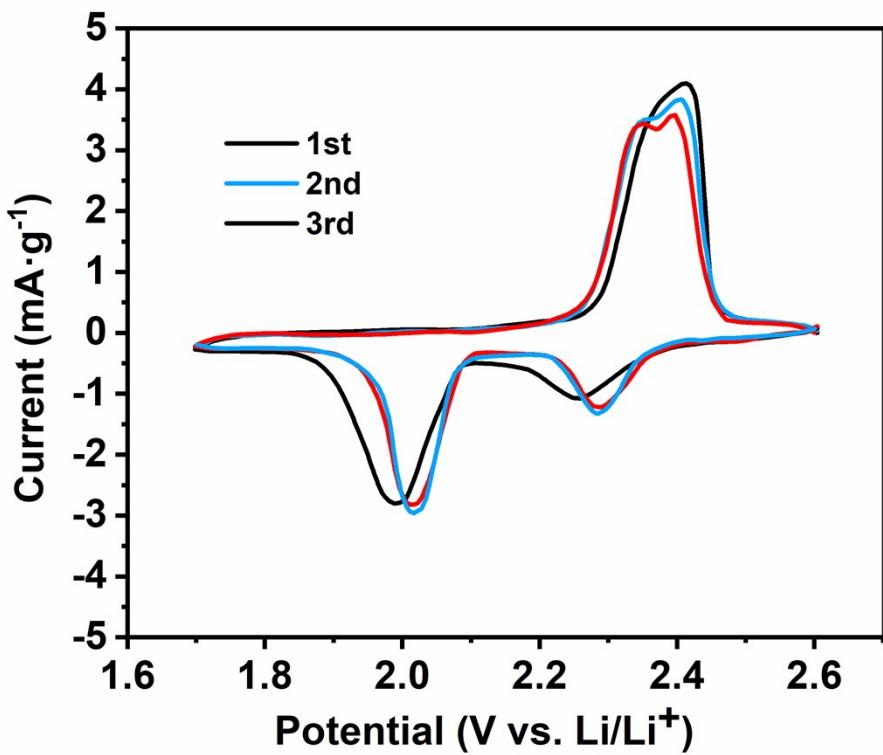


Figure S11 The C-V curve of $\text{V}_2\text{O}_5@\text{V}_2\text{C}$ of the initial 3 cycles.

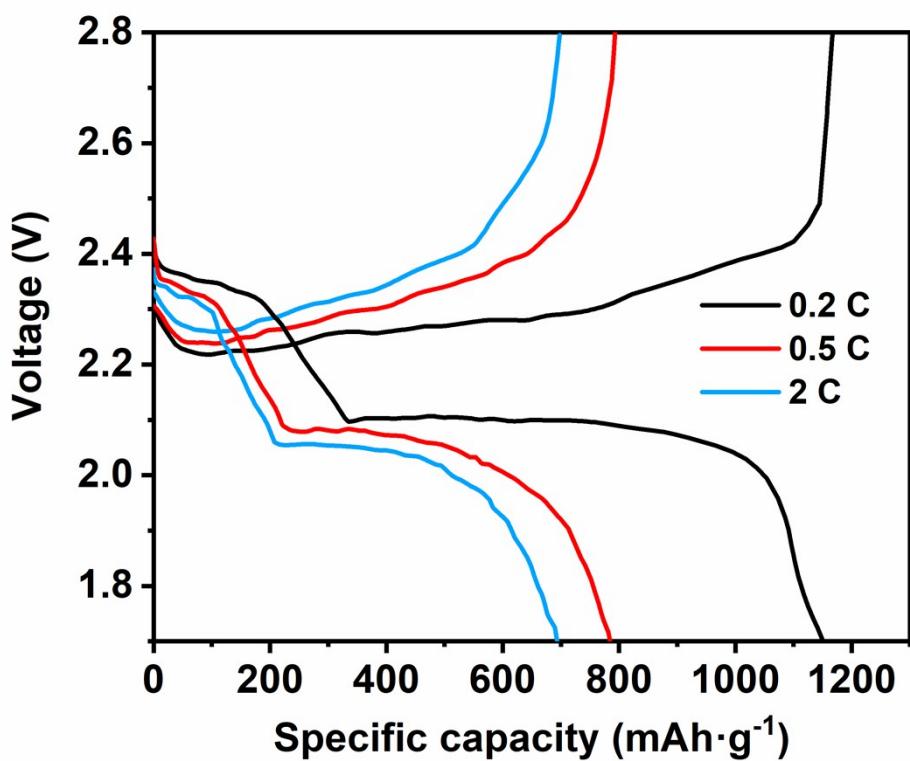


Figure S12 The charge and discharge curve of $\text{V}_2\text{O}_5@\text{V}_2\text{C}$.

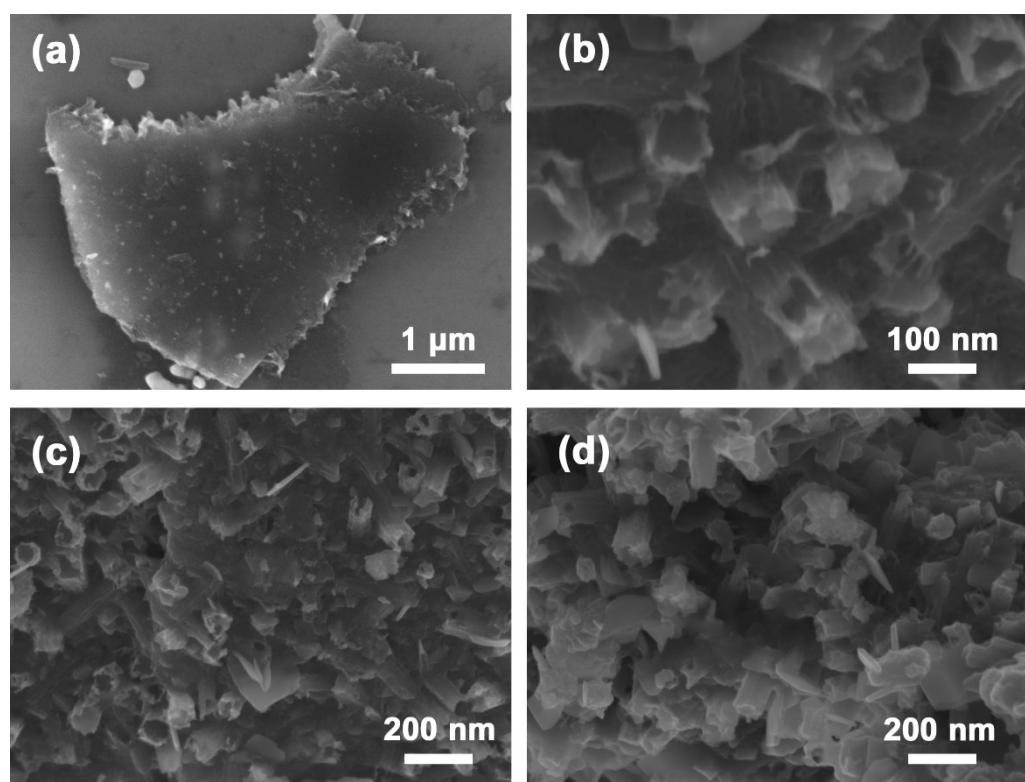


Figure S13 The SEM graph of (a) de- $\text{V}_2\text{O}_5@\text{V}_2\text{C}$ (b) $\text{V}_2\text{O}_5@\text{V}_2\text{C}$ after 100 cycles (c) $\text{V}_2\text{O}_5@\text{V}_2\text{C}$ after 500 cycles (d) $\text{V}_2\text{O}_5@\text{V}_2\text{C}$ after 1000 cycles.

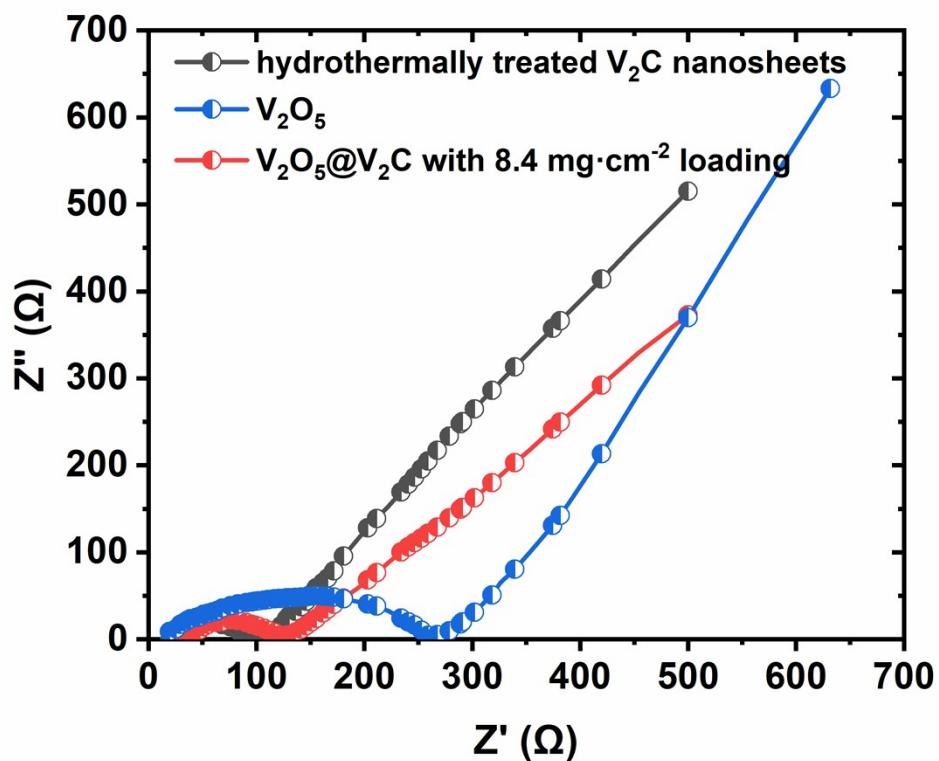


Figure S14 The EIS spectrum of V₂C, V₂O₅ and V₂O₅@V₂C with high S loading.

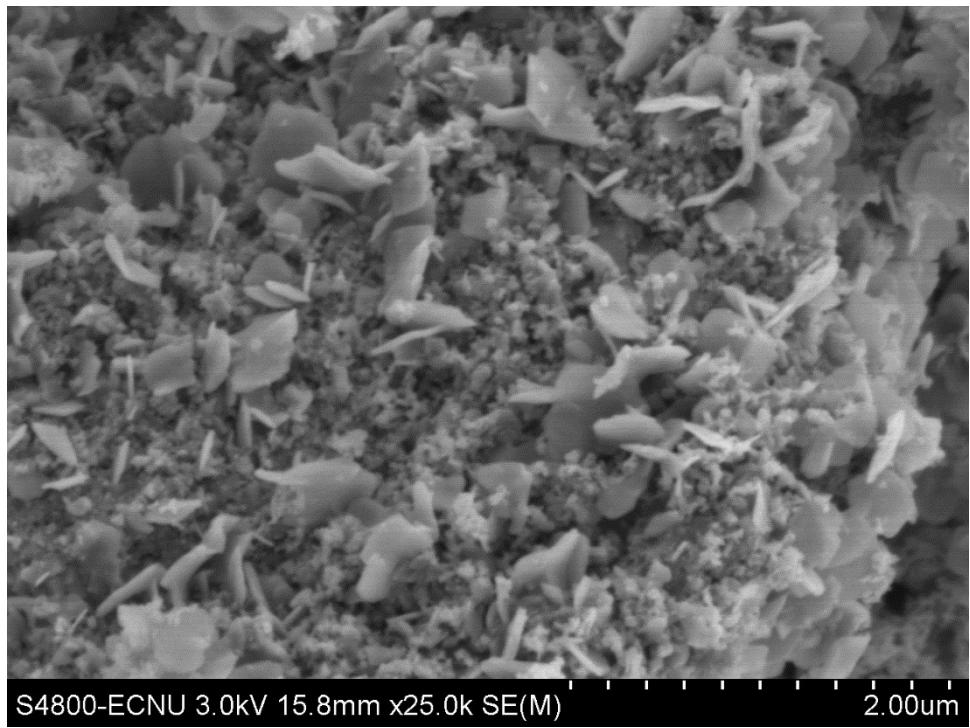


Figure S15 The $\text{V}_2\text{O}_5/\text{S}$ on Al foil.

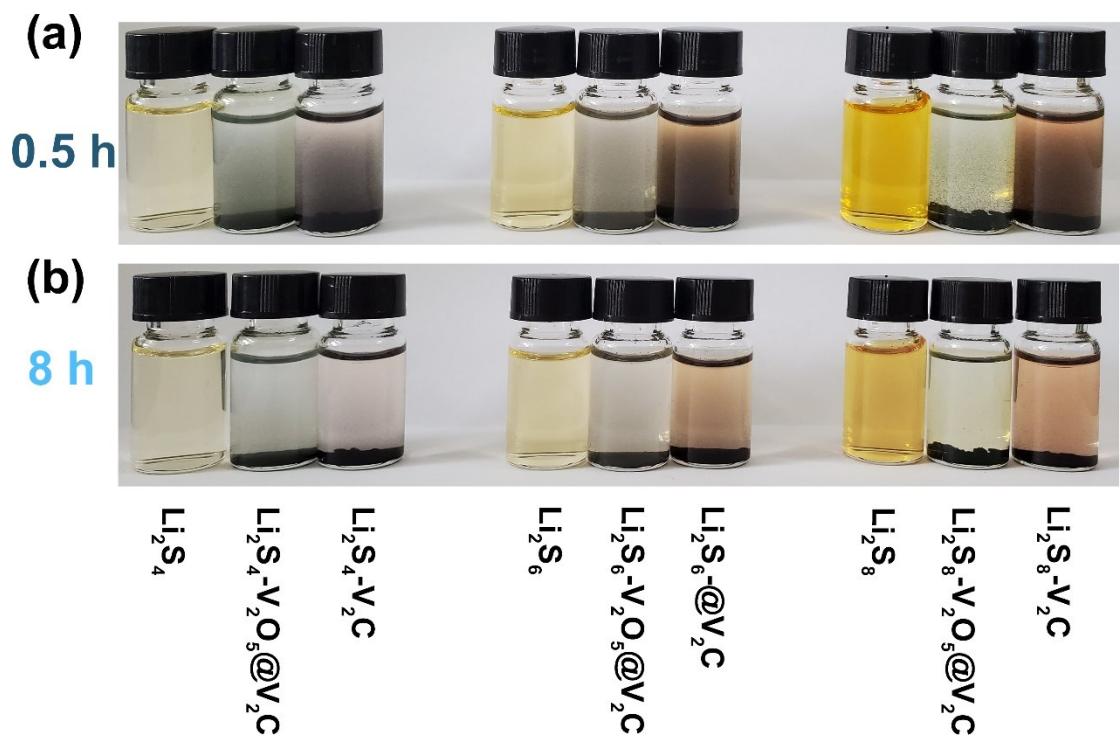


Figure S16 Adsorption performance test diagram of V_2C and $\text{V}_2\text{O}_5\text{@V}_2\text{C}$.

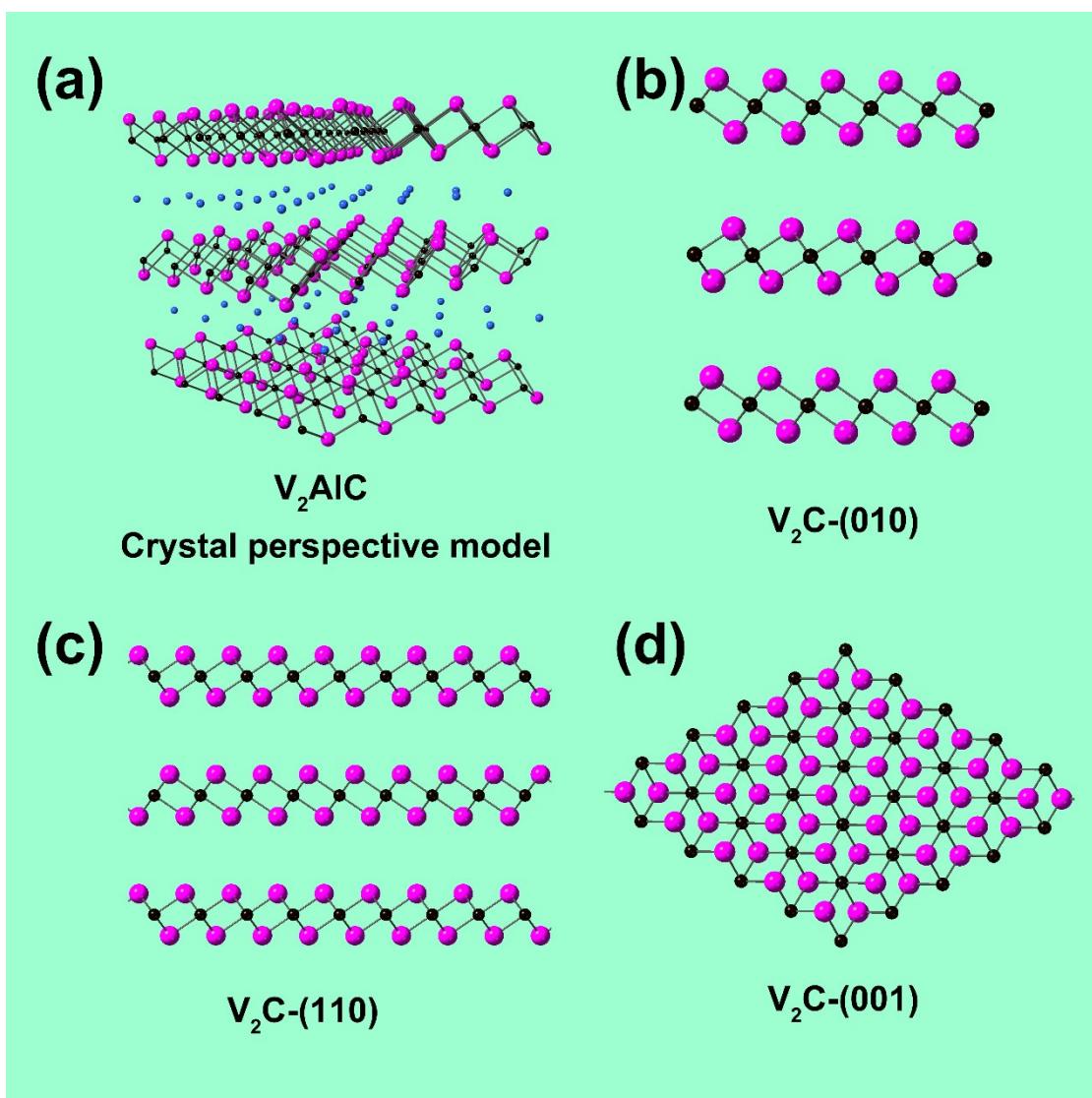


Figure S17 The crystal model of V₂AlC and V₂C.

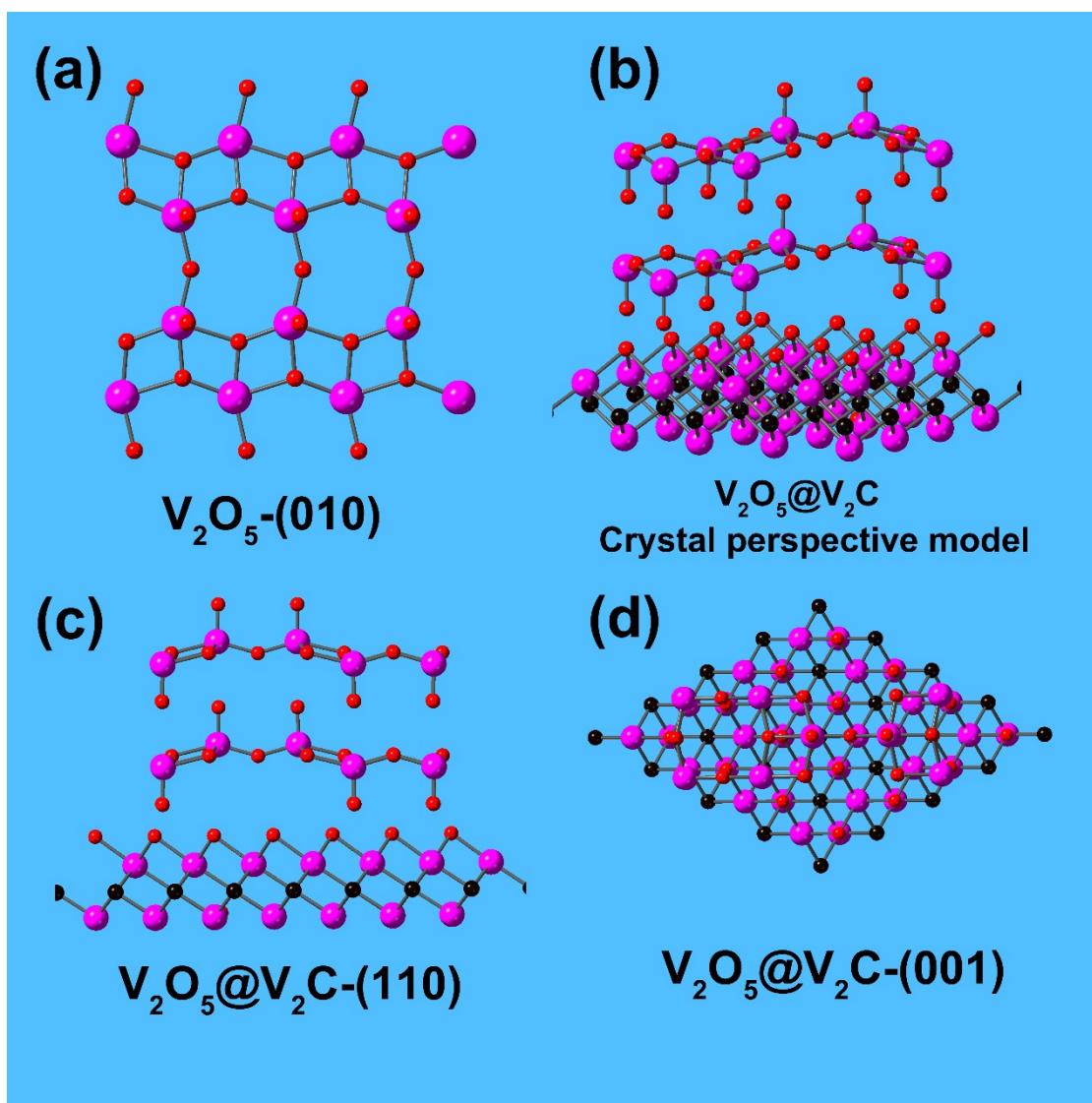


Figure S18 The crystal model of V_2O_5 and $\text{V}_2\text{O}_5@\text{V}_2\text{C}$.

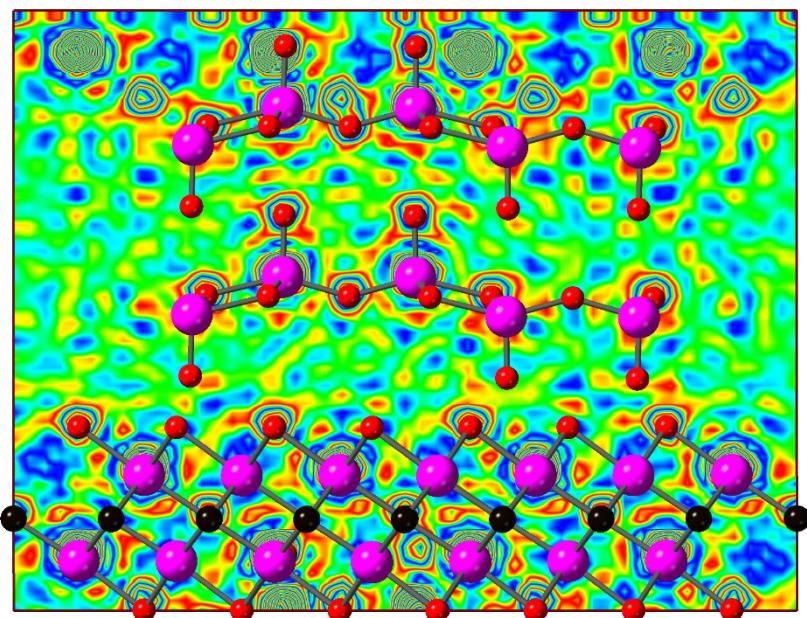


Figure S19 Regional charge density differential diagram of V₂O₅@V₂C.

Table S1. EDX distribution of V, O and C elements of pure V₂C, hydrothermally treated V₂C, V₂O₅@V₂C before and after cycling.

Element	Pure V ₂ C (at. %)	185°C hydrothermally treated V ₂ C (at. %)	de-V ₂ O ₅ @V ₂ C before cycling (at. %)	de-V ₂ O ₅ @V ₂ C after cycling (at. %)
V	62.74	53.07	57.83	56.42
C	35.11	22.89	25.36	25.03
O	2.15	24.04	16.81	18.55

Table S2 The surface energy of V₂O₅ with different crystal planes and the free

energy of the interface of V₂O₅@V₂C.

Lattice plane	XRD diffraction peak (°)	A (Å ²)	E _{slab} (10 ⁴ eV)	E _{bulk} (10 ⁴ eV)	E _{surf} (J/m ²)	V ₂ O ₅ @V ₂ C E _{free} (eV)	Interplanar crystal spacing (Å)
V ₂ O ₅ -(200)	15.35	15.54	-2.45674		0.2835	0.2761	5.768
V ₂ O ₅ -(001)	20.26	31.66	-2.45675		0.1419	0.2750	4.379
V ₂ O ₅ -(110)	26.13	26.30	-2.45528	-1.22840	0.2315	0.3816	3.408
V ₂ O ₅ -(301)	31.0	60.79	-2.45462		0.2876	1.0913	2.882
V ₂ C-(002)	8.50	68.20	-0.83330	-0.42217	1.2960	-	-

Table S3 Performance comparison table of vanadium base positive electrode matrix materials in recent years.

Host	S loading (mg cm⁻²)	Current density (C)	Cycles	Initial capacity (mAh g⁻¹)	Areal capacity (mAh cm⁻²)	Capacity decay (% per cycle)	Year	Ref
V₂O₅@V₂C	2.0	0.2	100	1173	2.35	0.043	-	This work
		0.5	1000	1138	2.28	0.047		
		2	500	1106	2.21	0.053		
	4.2	0.2	200	1093	4.50	0.078		
	8.4	0.2	200	1058	8.59	0.11		
VO ₂ (p)@V ₂ C	2.0	2	500	1210	2.42	0.062	2019	1
V ₂ O ₅ -rGO	1.2-1.5	0.2	300	~1000	1.2-1.5	0.048	2018	2
rGO-VS ₂	2.6	0.1	100	721	1.87	0.094	2018	3
VS ₂ -C	1-2	2	100	1185	1.18-2.37	0.16	2018	4
V ₂ O ₅ -C	5.5	2	500	790	1.6	0.041	2017	5
VO _x -SWCNT	1.0	1	300	1069	1.7	0.095	2018	6
VN-C	2.8	1	200	1200	2.8	0.24	2017	7
VN nanobubbles	6.8	0.5	200	800	5.4	0.15	2016	8
VO ₂ -VN	4.2	2	800	1105	2.21	0.06	2018	9

Table S4 Equivalent circuit fitting parameter result table.

Equivalent parameter	Initial		after cycling	
	V ₂ O ₅ @V ₂ C	V ₂ C	V ₂ O ₅ @V ₂ C	V ₂ C
R _s / Ohm	3.12	5.01	3.93	8.22
R _{surf} / Ohm	11.67	17.10	33.71	61.32
R _{ct} / Ohm	51.23	82.63	88.27	184.6

Table S5 Equivalent circuit fitting parameter result table.

Equivalent parameter	Hydrothermally treated V ₂ C	Pure V ₂ O ₅	V ₂ O ₅ @V ₂ C with 8.4 mg·cm ⁻² loading
R _s / Ohm	9.73	8.72	7.38
R _{surf} / Ohm	19.84	22.14	14.51
R _{ct} / Ohm	45.31	128.37	63.03

Reference

1. Z. Wang, K. Yu, Y. Feng, R. Qi, J. Ren and Z. Zhu, *ACS Appl. Mat. Interfaces*, 2019, **11**, 44282-44292.
2. Y. Guo, Y. Zhang, Y. Zhang, M. Xiang, H. Wu, H. Liu and S. Dou, *J. Mater. Chem. A*, 2018, **6**, 19358-19370.
3. Z. Cheng, Z. Xiao, H. Pan, S. Wang and R. Wang, *Adv. Energy Mater.*, 2018, **8**, 1702337
4. X. Zhu, W. Zhao, Y. Song, Q. Li, F. Ding, J. Sun, L. Zhang and Z. Liu, *Adv. Energy Mater.*, 2018, **8**, 1800201.
5. L. Ma, H. Yuan, W. Zhang, G. Zhu, Y. Wang, Y. Hu, P. Zhao, R. Chen, T. Chen, J. Liu, Z. Hu and Z. Jin, *Nano Lett.*, 2017, **17**, 7839-7846.
6. M. Zhang, Y. Yang, X. Zhang, M. Cheng, H. Yuan, K. Amin, A. Ahmad, L. Mao, W. Yan and Z. Wei, *Adv. Mater. Interfaces*, 2018, **5**, 1800766
7. X. Li, K. Ding, B. Gao, Q. Li, Y. Li, J. Fu, X. Zhang, P. K. Chu and K. Huo, *Nano Energy*, 2017, **40**, 655-662.
8. X. Liang, C. Y. Kwok, F. Lodi-Marzano, Q. Pang, M. Cuisinier, H. Huang, C. J. Hart, D. Houtarde, K. Kaup, H. Sommer, T. Brezesinski, J. Janek and L. F. Nazar, *Adv. Energy Mater.*, 2016, **6**, 1501636
9. Y. Song, W. Zhao, L. Kong, L. Zhang, X. Zhu, Y. Shao, F. Ding, Q. Zhang, J. Sun and Z. Liu, *Energy Environ. Sci.*, 2018, **11**, 2620-2630.