Supplementary Data

Rational design of MXene@TiO$_2$ nanoarray enabling dual lithium polysulfides chemisorption towards high-performance lithium-sulfur batteries

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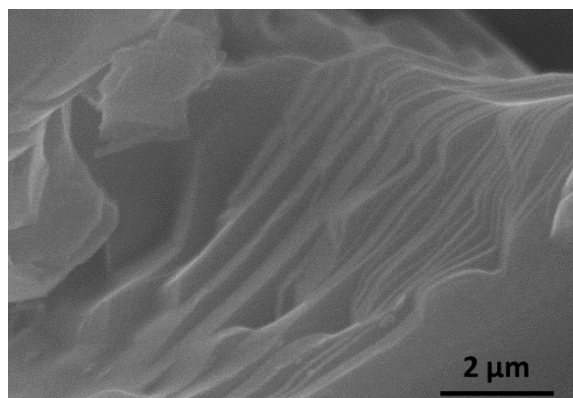
Supplementary Figures and Tables

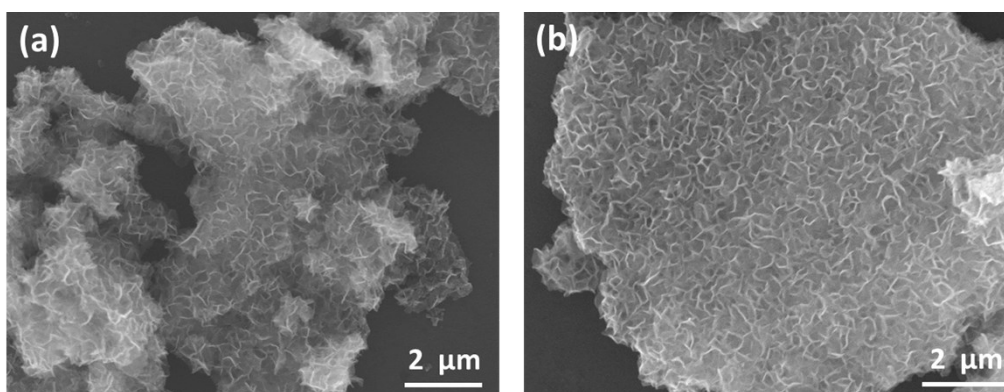**Fig. S1 SEM image of MAX precursor.**

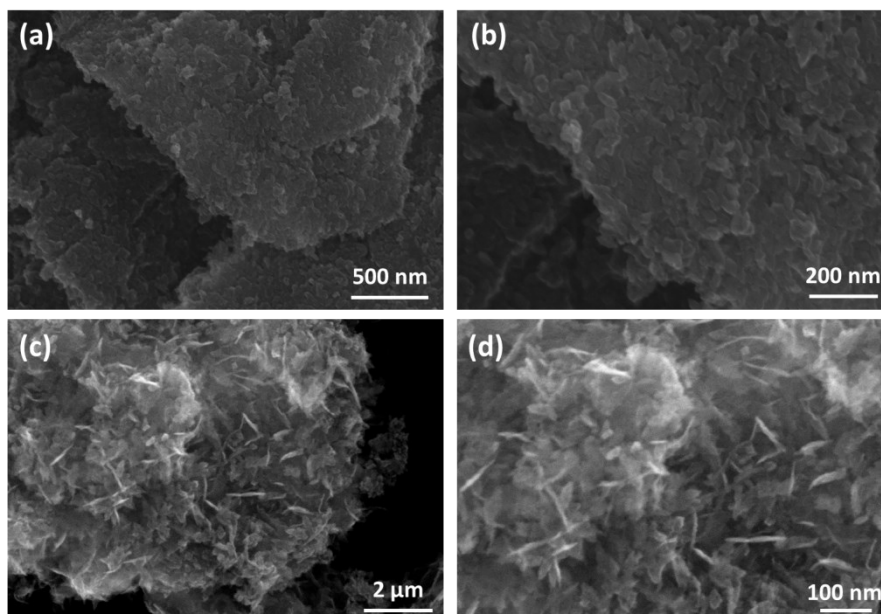**Fig. S2 Overall SEM images of MXene@TiO$_2$ nanoarray.**

Fig. S3 SEM images of MXene@TiO$_2$ composites with different inputs of titanium(IV) isopropoxide: (a, b) 0.6 mL; (c, d) 1.4 mL.

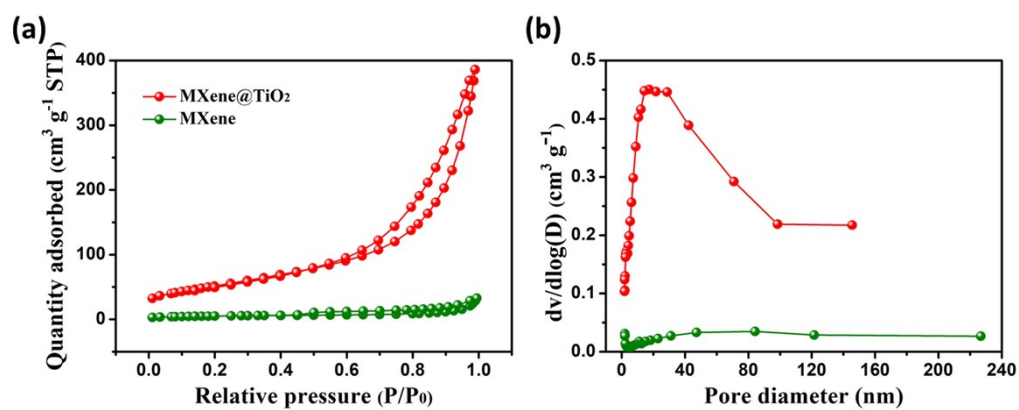**Fig. S4 (a) Nitrogen adsorption-desorption isotherms and (b) pore size distributions of MXene@TiO$_2$ nanoarray and individual MXene nanosheets.**
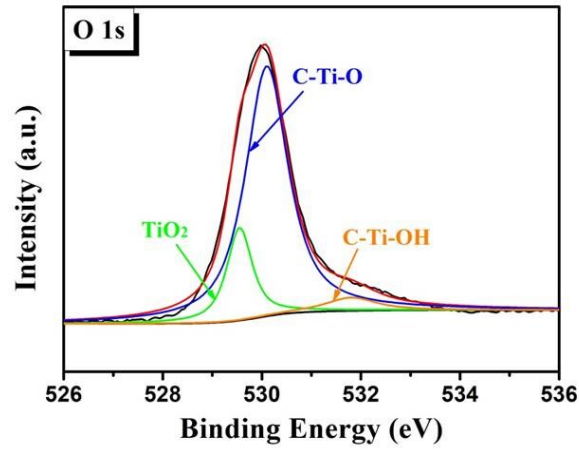
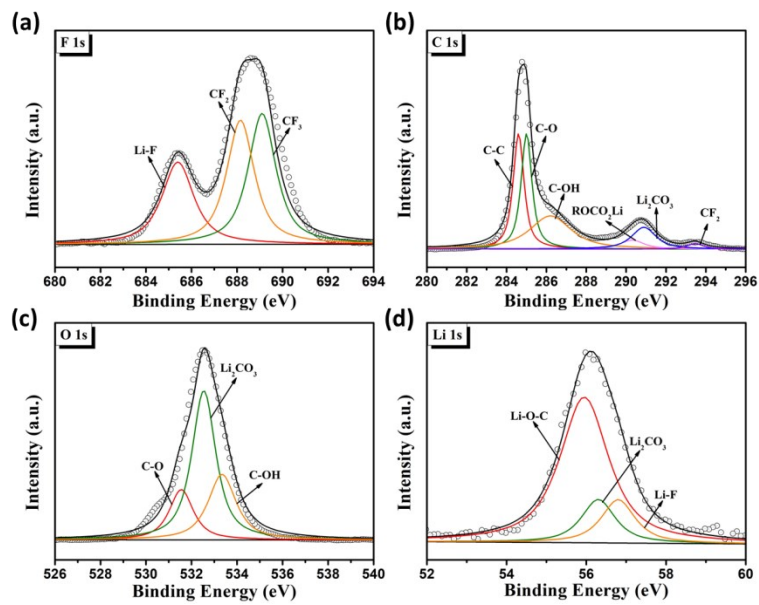**Fig. S5 O 1s XPS spectrum of MXene@TiO$_2$ nanoarray.**

Fig. S6 XPS spectra of MXene@TiO$_2$/S cathode surface after cycling: (a) F 1s; (b) C 1s; (c) O 1s; (d) Li 1s.
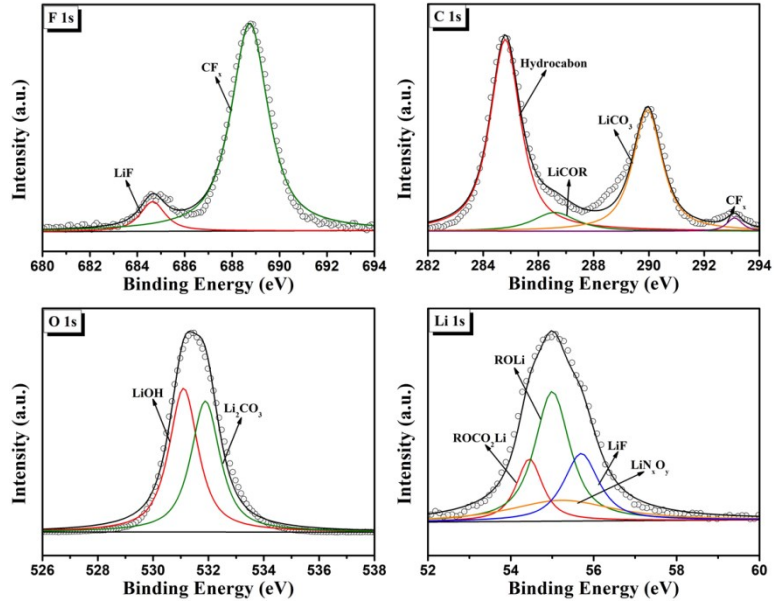
Fig. S7 XPS spectra of Li metal anode surface after cycling: (a) F 1s; (b) C 1s; (c) O 1s; (d) Li 1s.
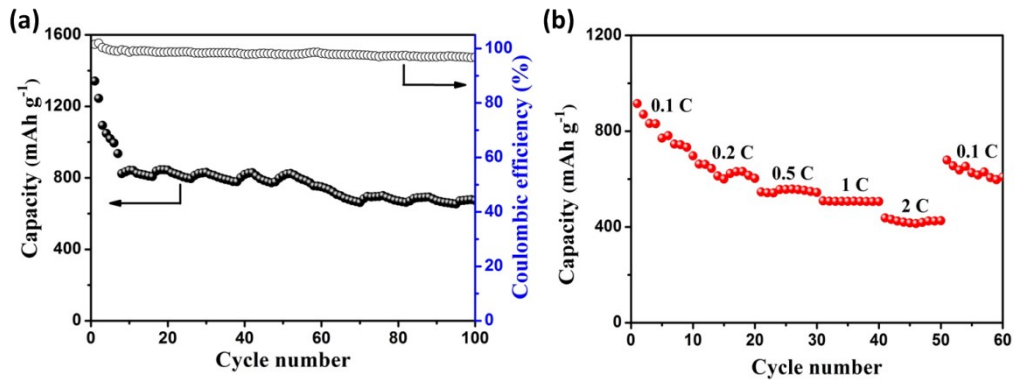

Fig. S8 (a) Cycling at 0.5 C and (b) rate performances of TiO$_2$/S cathode.

Fig. S9 Cycling behavior at 0.5 C of MXene@TiO$_2$/S cathode (sulfur loading=2.5 mg cm^{-2}).

Fig. S10 Nyquist plots of MXene@TiO$_2$/S, MXene/S and TiO$_2$/S cathodes with the equivalent circuit inset.

Fig. S11 UV-vis absorption spectra of Li_2S_4, MXene/Li_2S_4 and MXene@TiO_2/Li_2S_4 solutions after resting overnight. The digital photo inset shows the consequent color differences.

Fig. S12 Comparisons of second-circle CV curves at a scan rate of 0.2 mV s^{-1} between MXene@TiO_2/S and MXene/S cathodes.

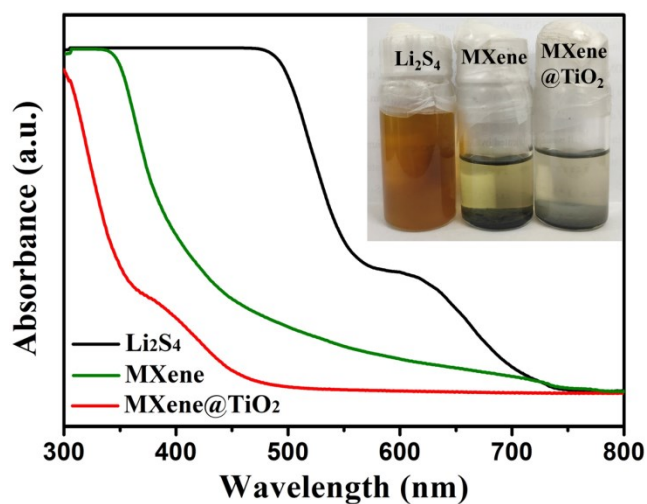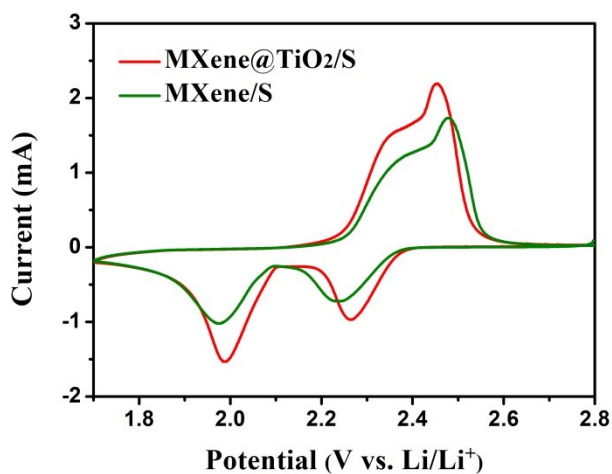**Table S1.** Elemental composition of MXene@TiO$_2$ nanoarray based on ICP-OES, C element analysis and stoichiometry.

Samples	C	Ti$_{(sum)}$	Ti$_{(MXene)}$	Ti$_{(TiO_2)}$
Wt%	6.24	65.13	37.30	27.83

Table S2. Electrochemical performance of Li-S batteries based on TiO$_2$- and MXene-based hosts.

Host materials	Sulfur (wt%)	Rate (C)	Cycle	Capacity (mAh g^{-1})	Ref.
MXene@TiO$_2$ nanoarray	71.2	0.5	100	1003.9	This work
MXene@TiO$_2$ nanoarray	71.2	2	500	612.7	This work
MC-Meso C-doped TiO$_2$	61.04	0.1	140	578	1
M2-GC-TiO$_2$	59	1	600	599	2
TiO$_2$/Ti$_2$C	78.4	2	200	464.0	3
GA/TiO$_2$	75.1	1	250	512	4
G–TiO$_2$	54	0.5	200	853.4	5
Ti$_3$C$_2$/CNT	79	0.5	1200	450	6
Ti$_3$C$_2$T$_x$/RGO	70.4	0.5	300	878.4	7
Ti$_2$C	70	0.5	650	723	8
MXene/1T-2H MoS$_2$-C	79.6	0.3	300	799.3	9
N-doped Ti$_3$C$_2$T$_x$	73.85	0.2	200	950	10

Table S3. Comparison of EIS fitting results for MXene@TiO$_2$/S, MXene/S and TiO$_2$/S cathodes.

Cathode materials	R$_e$(Ω)	R$_{int}$(Ω)	R$_{ct}$(Ω)
MXene@TiO$_2$/S	2.35	7.7	26.8
MXene/S	2.64	8.5	33.8
TiO$_2$/S	3.93	32.8	63.9

References

1 T. A. Zegeye, C.-F. J. Kuo, A. S. Wotango, C.-J. Pan, H.-M. Chen, A. M. Haregewoin, J.-H. Cheng, W.-N. Su and B.-J. Hwang, *J. Power Source*, 2016, **324**, 239.

2 G. D. Park, J. Lee, Y. Piao and Y. C. Kang, *Chem. Eng. J.*, 2018, **335**, 600.

3 C. Du, J. Wu, P. Yang, S. Li, J. Xu and K. Song, *Electrochim. Acta*, 2019, **295**, 1067.

4 J.-Q. Huang, Z. Wang, Z.-L. Xu, W. G. Chong, X. Qin, X. Wang and J.-K. Kim, *ACS Appl. Mater. Interfaces*, 2016, **8**, 28663.

5 H. Fan, Q. Tang, X. Chen, B. Fan, S. Chen and A. Hu, *Chem. Asian J.*, 2016, **11**, 2911.

6 X. Liang, Y. Rangom, C. Y. Kwok, Q. Pang and L. F. Nazar, *Adv. Mater.*, 2016, **29**, 1603040.

7 W. Bao, X. Xie, J. Xu, X. Guo, J. Song, W. Wu, D. Su and G. Wang, *Chem. Eur J.*, 2017, **23**, 12613.

8 X. Liang, A. Garsuch and L. F. Nazar, *Angew. Chem. Int. Ed.*, 2015, **54**, 3907.

9 Y. Zhang, Z. Mu, C. Yang, Z. Xu, S. Zhang, X. Zhang, Y. Li, J. Lai, Z. Sun, Y. Yong, Y. Chao, C. Li, X. Ge, W. Yang and S. Guo, *Adv. Funct. Mater.*, 2018, **28**, 1707578.

10 W. Bao, L. Liu, C. Wang, S. Choi, D. Wang and G. Wang, *Adv. Energy Mater.*, 2018, **8**, 1702485.