Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Supporting information

Improving the Performance of Titanium Carbide MXene in Supercapacitor by Partial Oxidation Treatment

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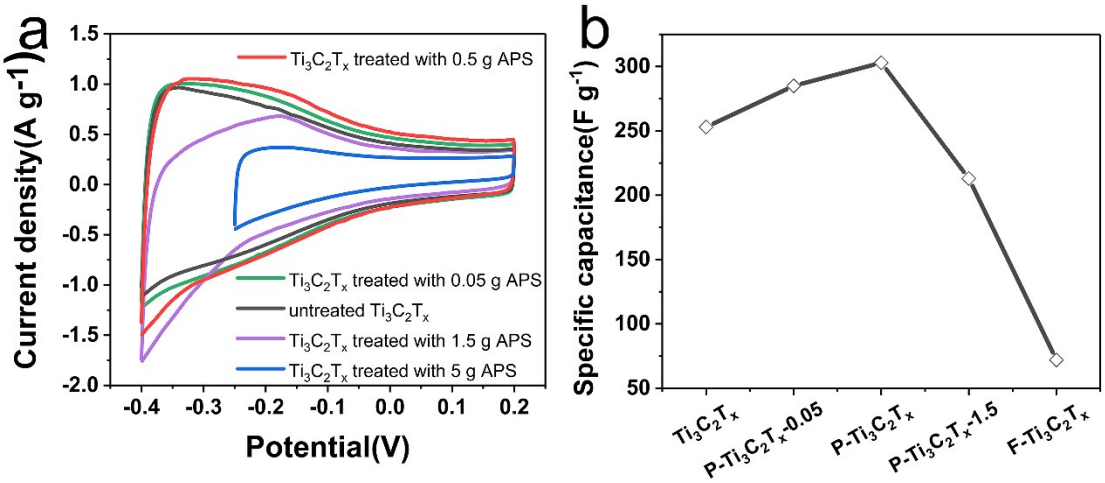

Figure S1. CV curves of the different $Ti_3C_2T_x$ samples at 2 mV s^{-1}. 50 mL of 4 mg mL^{-1} $Ti_3C_2T_x$ was treated with 0.5, 0.05, 1.5, 5 g ammonium persulfate, respectively. (b) the specific capacitance of the different $Ti_3C_2T_x$ samples.

Table S1. ICP analysis results of the Al in the Ti_3AlC_2 and $Ti_3C_2T_x$.

sample	Al (mg/kg)	wt.%
Ti_3AlC_2	128428	12.843
$Ti_3C_2T_x$	7954	0.795

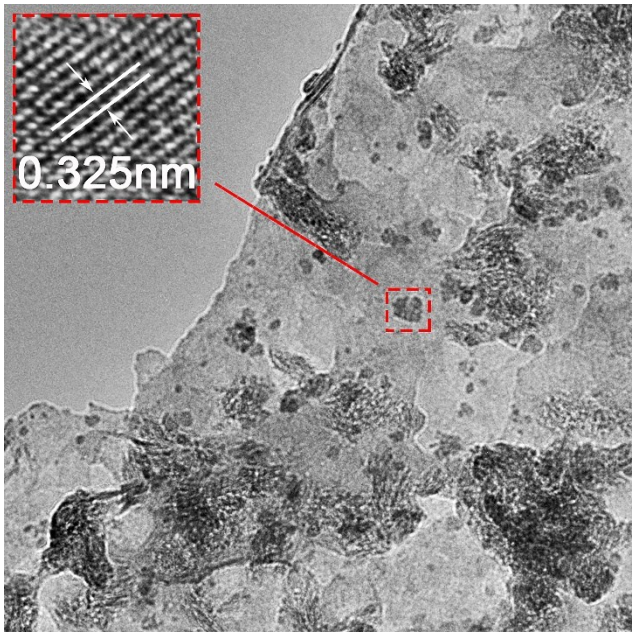

Figure S2. HRTEM image of the F-$Ti_3C_2T_x$ sample.

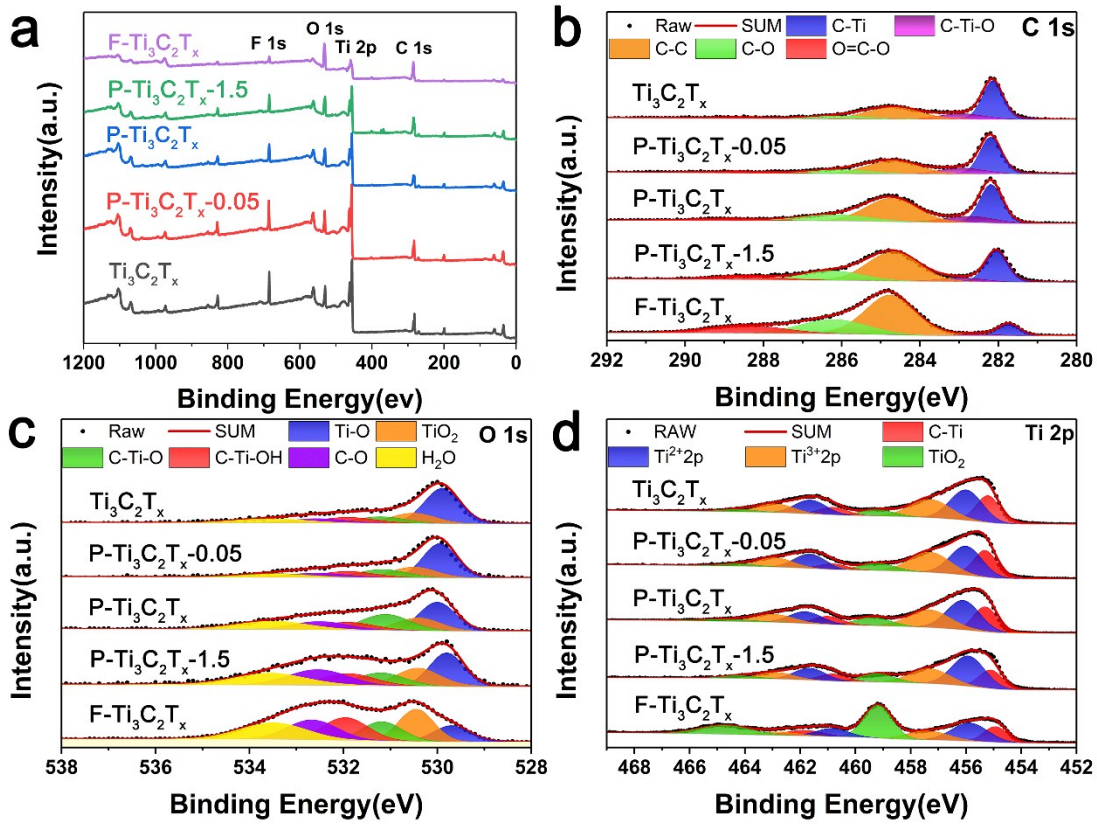

Figure S3. (a) XPS survey spectra of $Ti_3C_2T_x$, P-$Ti_3C_2T_x$-0.05, P-$Ti_3C_2T_x$, P-$Ti_3C_2T_x$-1.5 and F-$Ti_3C_2T_x$. High-resolution C 1s (b), O 1s (c), and Ti 2p (d) XPS spectra of $Ti_3C_2T_x$, P-$Ti_3C_2T_x$-0.05, P-$Ti_3C_2T_x$, P-$Ti_3C_2T_x$-1.5 and F-$Ti_3C_2T_x$ samples.

High-resolution C 1s spectra (Figure S3b) and Ti 2p spectra (Figure S3d) reveals that the C–Ti signal of P-$Ti_3C_2T_x$-0.5 and P-$Ti_3C_2T_x$ had no significant change, but the intensity of C–Ti signal signal obviously decreased in the P-$Ti_3C_2T_x$-0.5 and F-$Ti_3C_2T_x$ samples after treatment with excessive ammonium persulfate. Meanwhile, the high-resolution O1s spectra (Figure S3c) and Ti 2p spectra (Figure S3d) show a much stronger TiO_2 peak in F-$Ti_3C_2T_x$, when compared with untreated $Ti_3C_2T_x$. In particular, in Figure S3c, the high-resolution O 1s spectra of the partially oxidized $Ti_3C_2T_x$ possessed a much stronger C–Ti–O signal, confirming that the –O terminal could be formed in the partial oxidation treatment method.

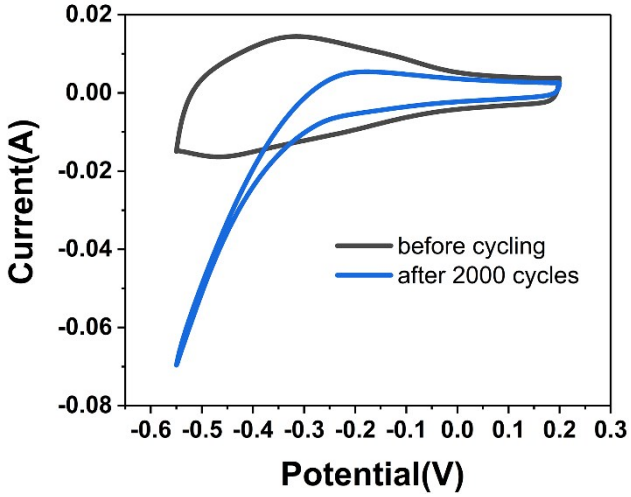

Figure S4. The cycling stability of P-$Ti_3C_2T_x$ in range of −0.55V ~ 0.2V at 5 mV s^{-1}.

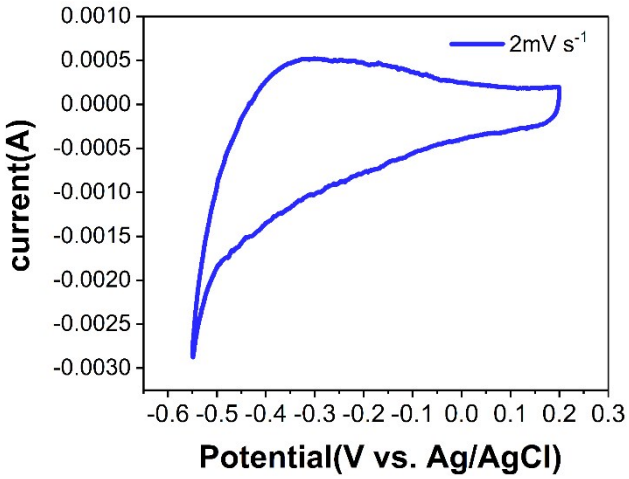

Figure S5. CV curves of the F-$Ti_3C_2T_x$ sample from −0.55 to 0.2 V. Obvious hydrogen evolution reaction can be observed in F-$Ti_3C_2T_x$ electrode near −0.4 V.

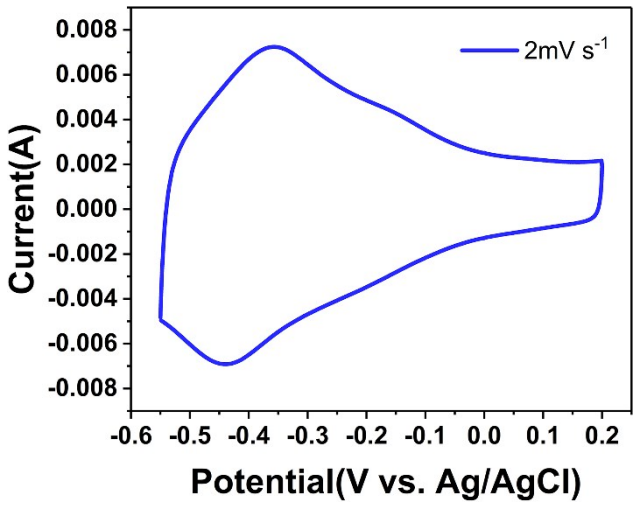

Figure S6. CV curves of the P-$Ti_3C_2T_x$ sample from −0.55 to 0.2 V. It is noted that no hydrogen

evolution reaction could be observed near −0.4 V.

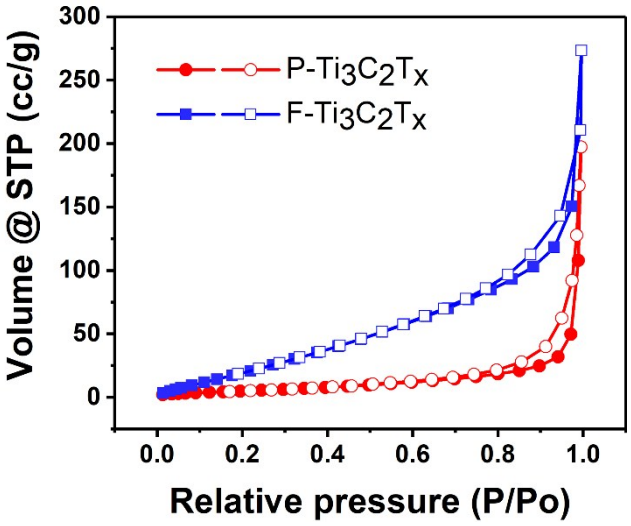

Figure S7. The nitrogen adsorption and desorption isotherms of the P-$Ti_3C_2T_x$ and F-$Ti_3C_2T_x$ samples.

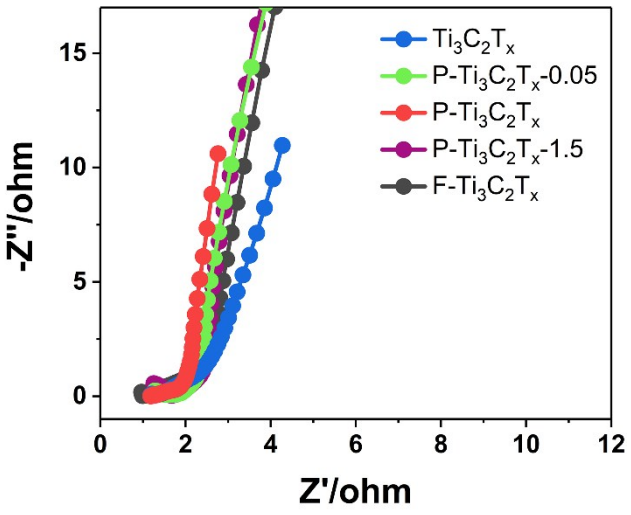

Figure S8. Nyquist plots for the different $Ti_3C_2T_x$ electrodes at open circuit potentials.

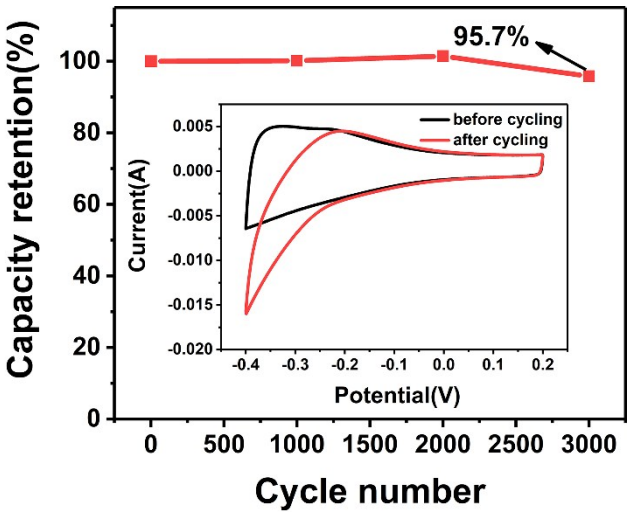

Figure S9. Cycle life performance of the $Ti_3C_2T_x$ electrode in 1 M H_2SO_4 electrolyte at 500 mV s^{-1}.

The inset shows the CV curves before and after cycling at 5 mV s^{-1}.

Table S2. Performance comparison of the electrochemical supercapacitors with other works.

Electrode material	Electrolyte	Capacitance	Cycling stability	Ref.
P-$Ti_3C_2T_x$	1 M H_2SO_4	303 F/g (2 mV/s)	96.6%/9000 cycles	In this work
TiO_2-Ti_3C_2	6 M KOH	143 F/g (5 mV/s)	96%/3000 cycles	1
$Ti_3C_2T_x$(via Alkali Treatment)	1 M H_2SO_4	314 F/g (2 mV/s)	89.1%/10 000 cycles	2
$Ti_3C_2T_x$	1 M H_2SO_4	150 F/g (2 mV/s)	No reported	3
$Ti_3C_2T_x$-15M	1 M H_2SO_4	192 F/g (2 mV/s)	No reported	4
PANI@TiO_2/$Ti_3C_2T_x$	1 M KOH	188.3 F/g (10 mV/s)	94%/8000 cycles	5
Ti_3C_2 film	3 M H_2SO_4	210 F/g (10 V/s)	90%/10000 cycles	6
Ti_3C_2/TiO_2–nanowires	6 M KOH	143 F/g (2 mV/s)	88%/6000 cycles	7
hydrazine-treated $Ti_3C_2T_x$	1 M H_2SO_4	250 F/g (2 mV/s)	≈100%/10000 cycles	8
Functionalized-Ti_3C_2	1M KOH	160 F/g (5 mV/s)	91%/10000 cycles	9

Reference

1. JianFeng Zhu, Yi Tang, ChenHui Yang, Fen Wang, and MinJuan Cao, Composites of TiO_2 Nanoparticles Deposited on Ti_3C_2 MXene Nanosheets with Enhanced Electrochemical Performance, *J. Electrochem. Soc.*, 2016,**163**,A785-A791.
2. T. Li, L. Yao, Q. Liu, J. Gu, R. Luo, J. Li, X. Yan, W. Wang, P. Liu, B. Chen, W. Zhang, W. Abbas, R. Naz and D. Zhang, Fluorine-Free Synthesis of High-Purity $Ti_3C_2T_x$(T=OH, O) via Alkali Treatment, *Angew. Chem.-Int. Edit.*, 2018, **57**, 6115-6119.
3. Y. Dall'Agnese, M. R. Lukatskaya, K. M. Cook, P.-L. Taberna, Y. Gogotsi and P. Simon, High capacitance of surface-modified 2D titanium carbide in acidic electrolyte, *Electrochem.*

Commun., 2014, **48**, 118-122.

4. M. Hu, T. Hu, Z. Li, Y. Yang, R. Cheng, J. Yang, C. Cui and X. Wang, Surface Functional Groups and Interlayer Water Determine the Electrochemical Capacitance of $Ti_3C_2T_x$ MXene, *ACS Nano*, 2018, **12**, 3578-3586.
5. X. Lu, J. Zhu, W. Wu and B. Zhang, Hierarchical architecture of PANI@TiO_2/$Ti_3C_2T_x$ ternary composite electrode for enhanced electrochemical performance, *Electrochim. Acta*, 2017, **228**, 282-289.
6. M. R. Lukatskaya, S. Kota, Z. Lin, M.-Q. Zhao, N. Shpigel, M. D. Levi, J. Halim, P.-L. Taberna, M. W. Barsoum, P. Simon and Y. Gogotsi, Ultra-high-rate pseudocapacitive energy storage in two-dimensional transition metal carbides, *Nature Energy*, 2017, **2**, 17105.
7. M. J. Cao, F. Wang, L. Wang, W. L. Wu, W. J. Lv and J. F. Zhu, Room Temperature Oxidation of Ti_3C_2 MXene for Supercapacitor Electrodes, *J. Electrochem. Soc.*, 2017, **164**, A3933-A3942.
8. O. Mashtalir, M. R. Lukatskaya, A. I. Kolesnikov, E. Raymundo-Pinero, M. Naguib, M. W. Barsoum and Y. Gogotsi, The effect of hydrazine intercalation on the structure and capacitance of 2D titanium carbide (MXene), *Nanoscale*, 2016, **8**, 9128-9133.
9. H. Wang, J. Zhang, Y. Wu, H. Huang and Q. Jiang, Chemically functionalized two-dimensional titanium carbide MXene by in situ grafting-intercalating with diazonium ions to enhance supercapacitive performance, *J. Phys. Chem. Solids*, 2018, **115**, 172-179.