Supporting Information

Synthesis of Analogues Urchined Rutile Titania Carbon Nanocomposites by Iron-facilitated Phase Transformation of MXene for Environmental Remediation

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Table S1. The summarized Cr(VI) removal capacity, mechanism and condition of TiO2 materials reported previously

TiO_2 crystal	Cr(VI) removal capacity	mechanism	Conditions	Reference
Mesoporous TiO_2 (anatase)	33.2mg/g	Adsorption	pH=6-8, 298K	S1
Amorphous hydrous TiO2	4.8 mg/g	Adsorption	pH=2	S2
TiO_2-MCM-41 (anatase)	6.24mg/g	Adsorption	NA	S3
C/TiO_2 hybrid microsphere	18.1mg/g	Adsorption	pH=7, 298K	S4
Fe_3O_4@mTiO_2@GO microspheres	67.3 mg/g	Adsorption	pH=2, 303K	S5
Anatase TiO_2 hollow spheres	23 mg/g	Adsorption	pH=2.7, 298K	S6
High surface area TiO_2 (anatase)	6.98 mg/g	Adsorption	NA	S7
Peroxide-modified TiO2 (anatase)	63.5 mg/g	Adsorption	pH=5.0	S8
TiO_2 superstructure with ultrathin rutile nanorods	1000 mg/g	Photocatalysis	Sunlight for 3h	S9
Sulfated TiO_2 (anatase)	3.55 mg/g	Adsorption + Photocatalysis	**NA**	S10
Hierarchical structure TiO_2 hollow spheres	50 mg/g	Photocatalysis	4 h of UV irradiation	S11
u-RTC	**225 mg/g**	**Adsorption**	**pH= 5.8-6.5, 298K**	**Present study**

References

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S11 Yang, Y.; Wang, G.; Deng, Q.; Wang, H.; Zhang, Y.; Ng, D. H.; Zhao, H. Enhanced photocatalytic activity of hierarchical structure TiO_2 hollow spheres with reactive (001) facets for the removal of toxic heavy metal Cr (VI). *RSC Advances* 2014, 4, 34577-34583.

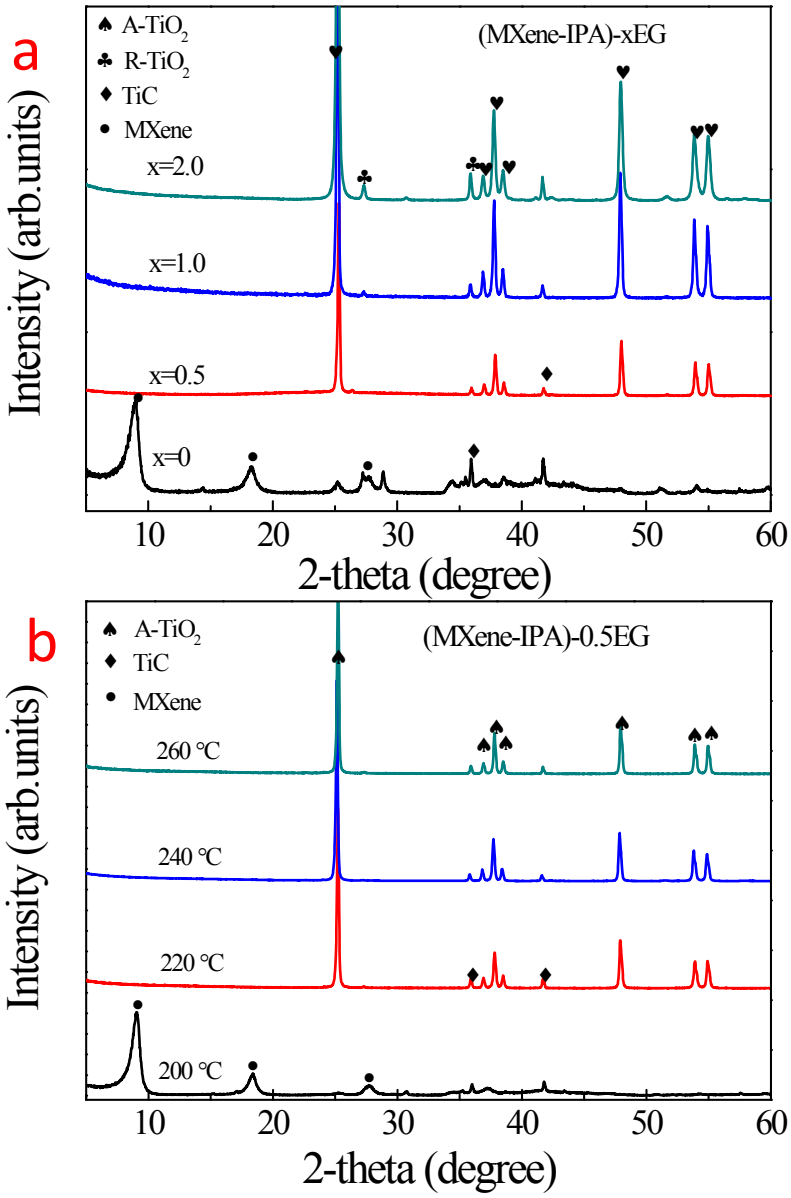

Figure S1. XRD patterns of different samples. (a) at 220℃ under different EG concentrations; (b) at different temperatures with 0.5EG.

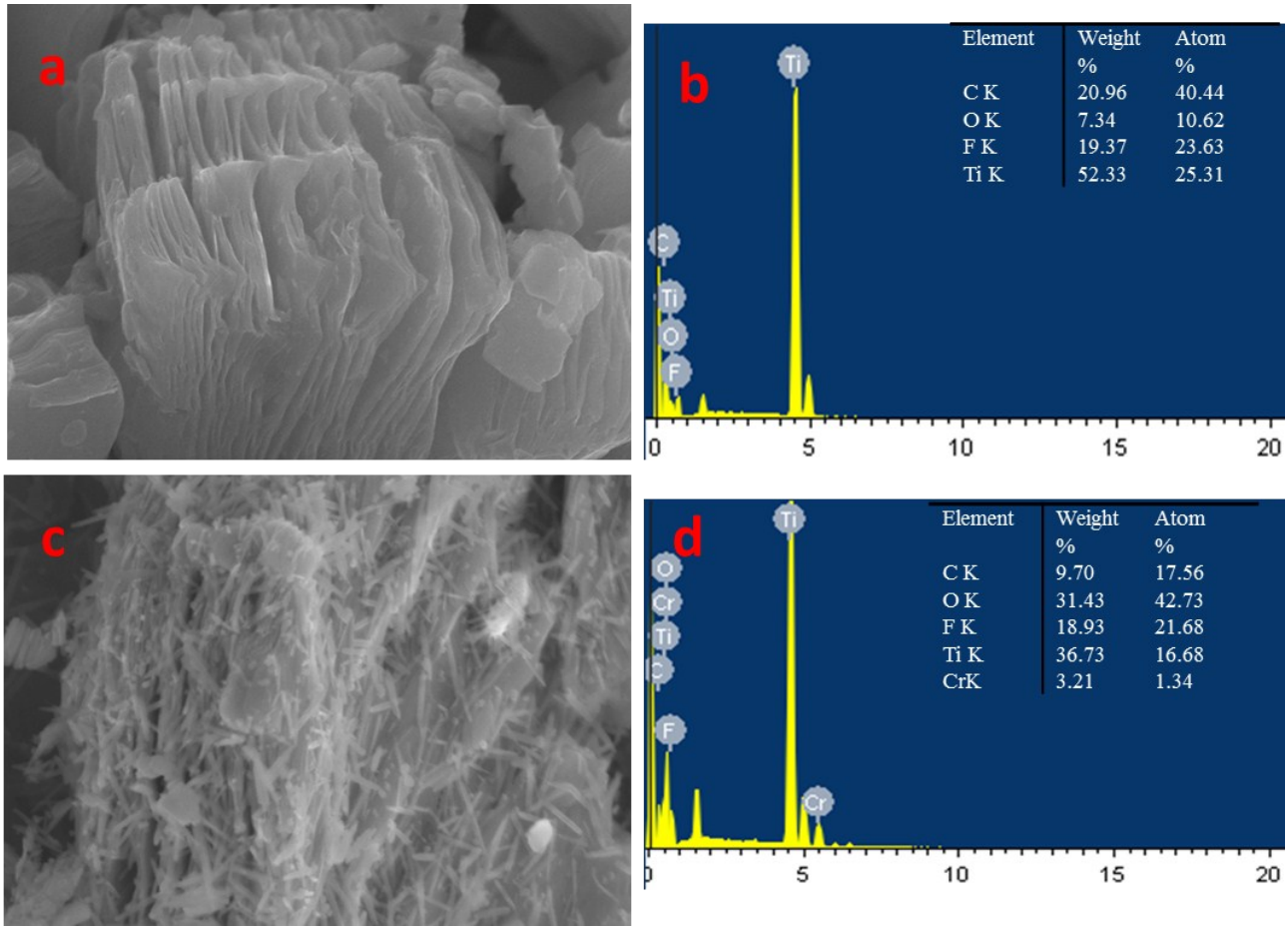

Figure S2. (a) and (b) The morphology of MXene and its chemical composition, respectively. (c) and (d) The morphology of u-RTC after removing Cr and its chemical composition. respectively.

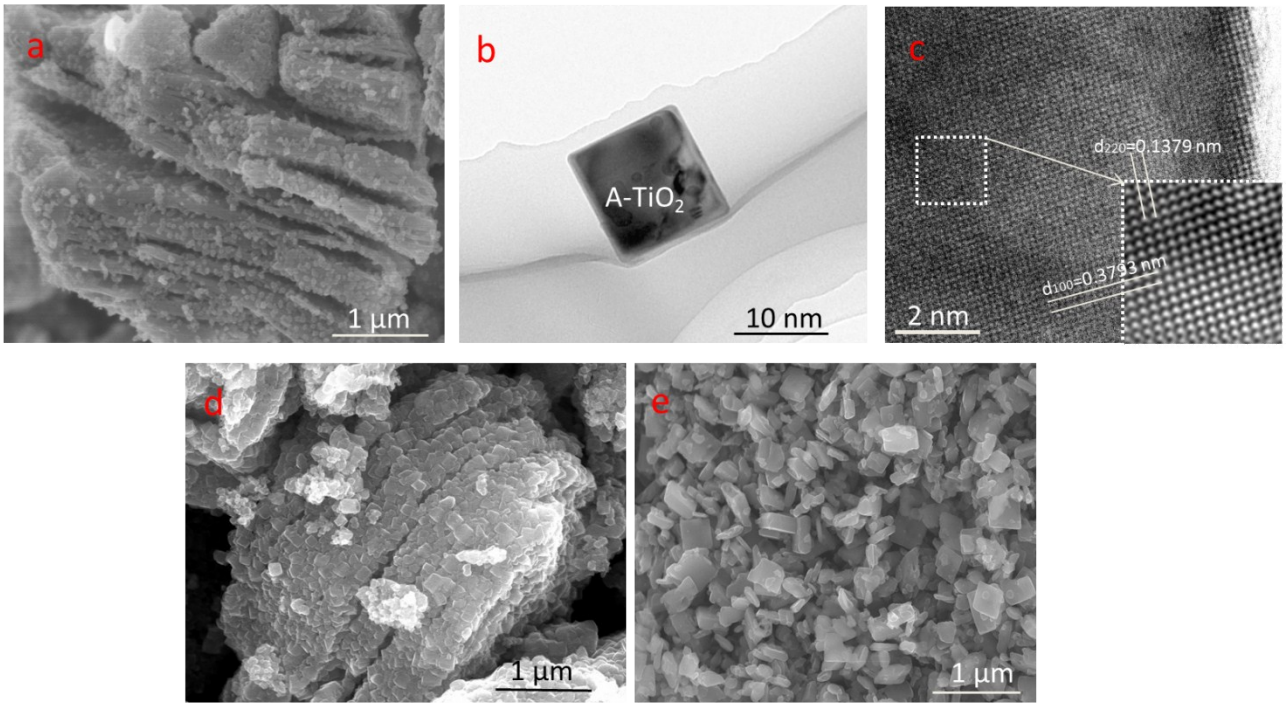

Figure S3. The morphology variation during decomposition of MXene at 220 ℃. (a) The SEM image of (MXene-IPA)-0.5EG for 1 h. (b) and (c) The TEM and HRTEM images of (MXene-IPA)-0.5EG for 1 h, respectively. (d) The SEM image of (MXene-IPA)-0.5EG for 4 h. (e) The SEM image of (MXene-IPA)-0.5EG for 24 h.

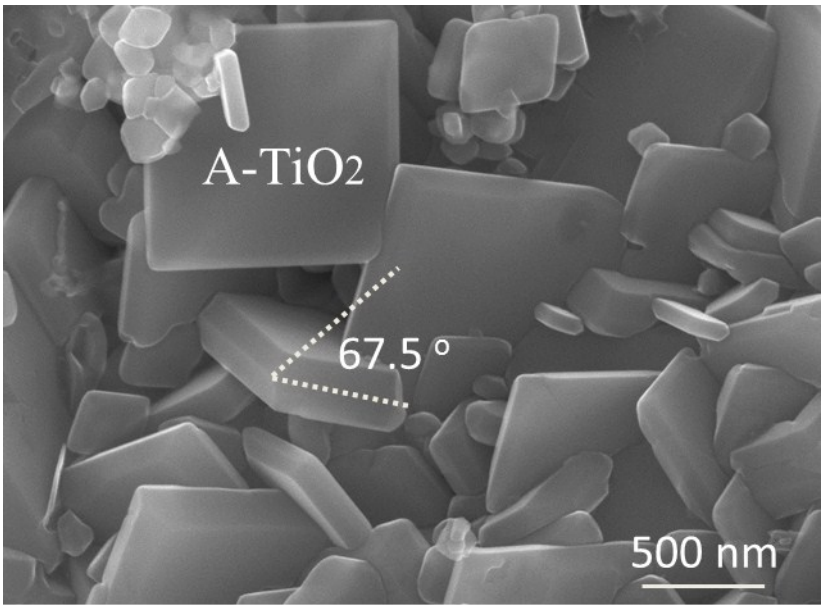

Figure S4. The SEM image of (MXene-IPA)-0.5EG for 28 h, which is similar to that of 24 h. The white dash lines indicate the (001) and (101) crystal planes of A-TiO_2, respectively. The angle is 67.5 ±0.5° on average.

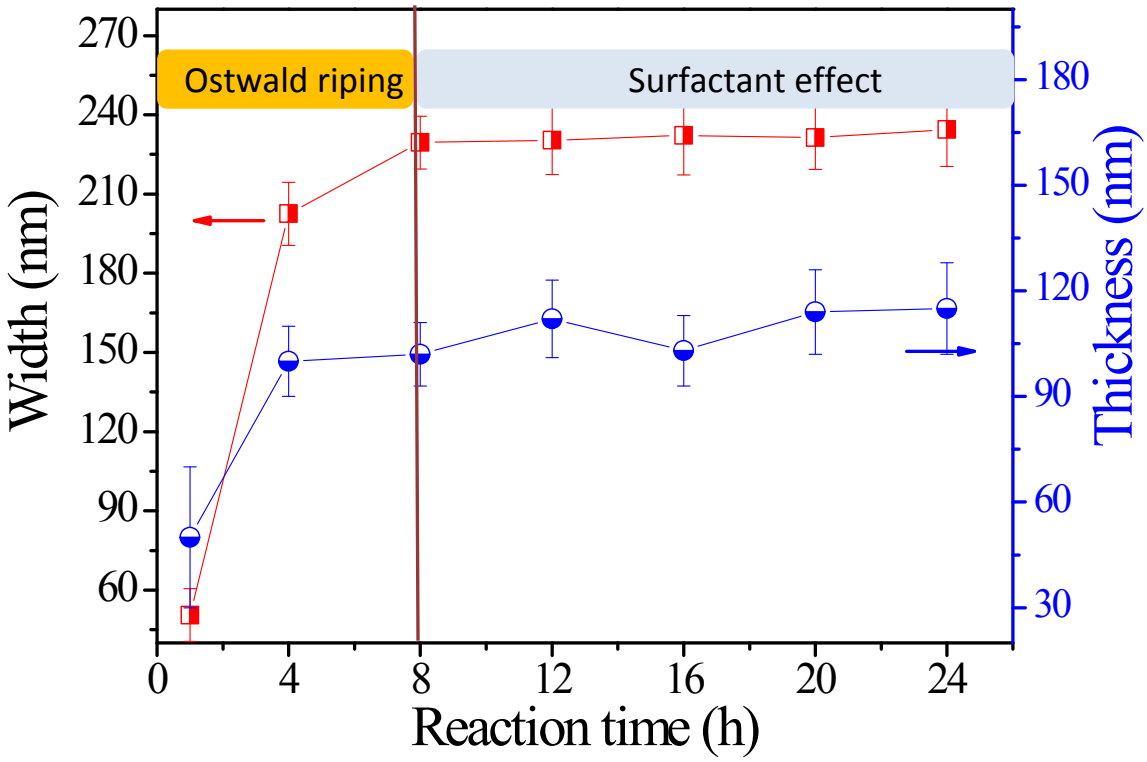

Figure S5. The effect of reaction time on the width and thickness of anatase TiO_2 in (MXene-IPA)-0.5EG.

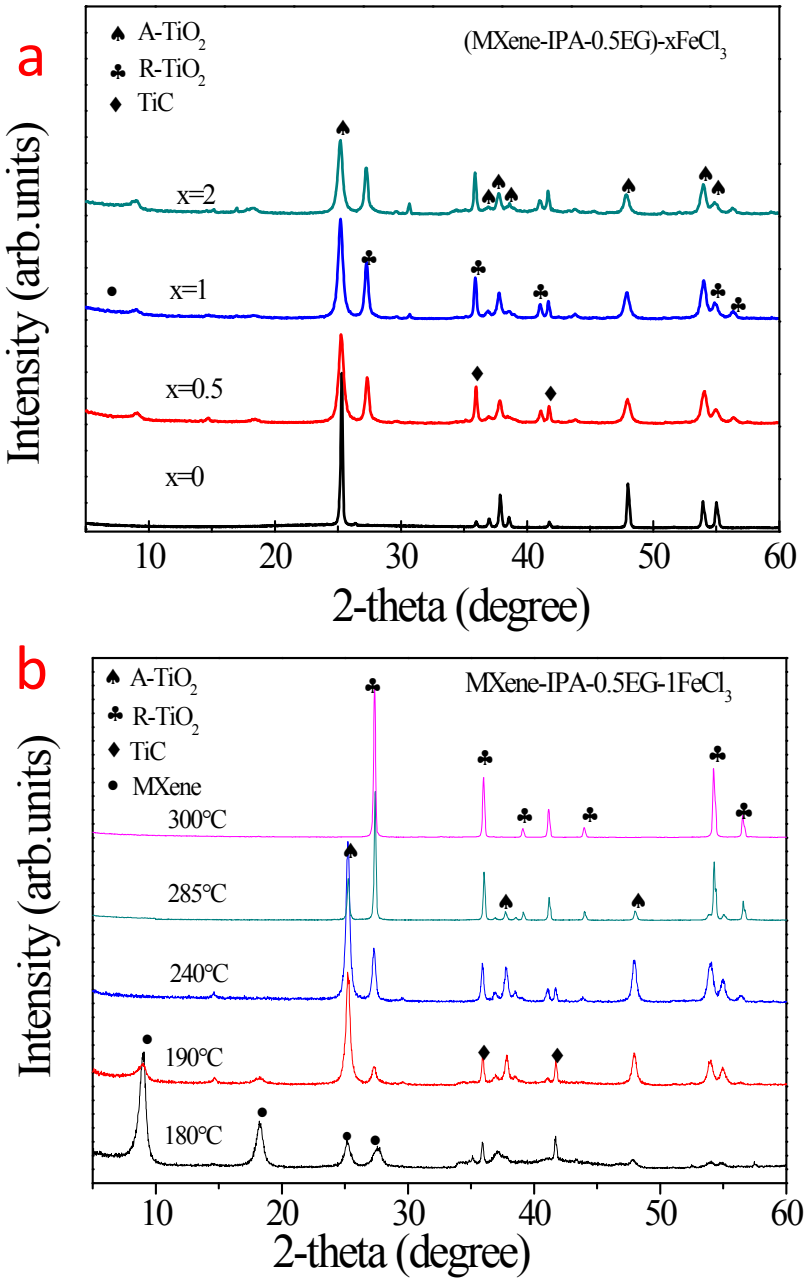

Figure S6. The representative XRD patterns. (a) The effect of $FeCl_3$ concentrations on the phase composition of decomposed MXene at 220 ℃ for 24 h. (b) The effect of reaction temperatures on the phase composition of decomposed MXene with 0.5EG for 24 h.

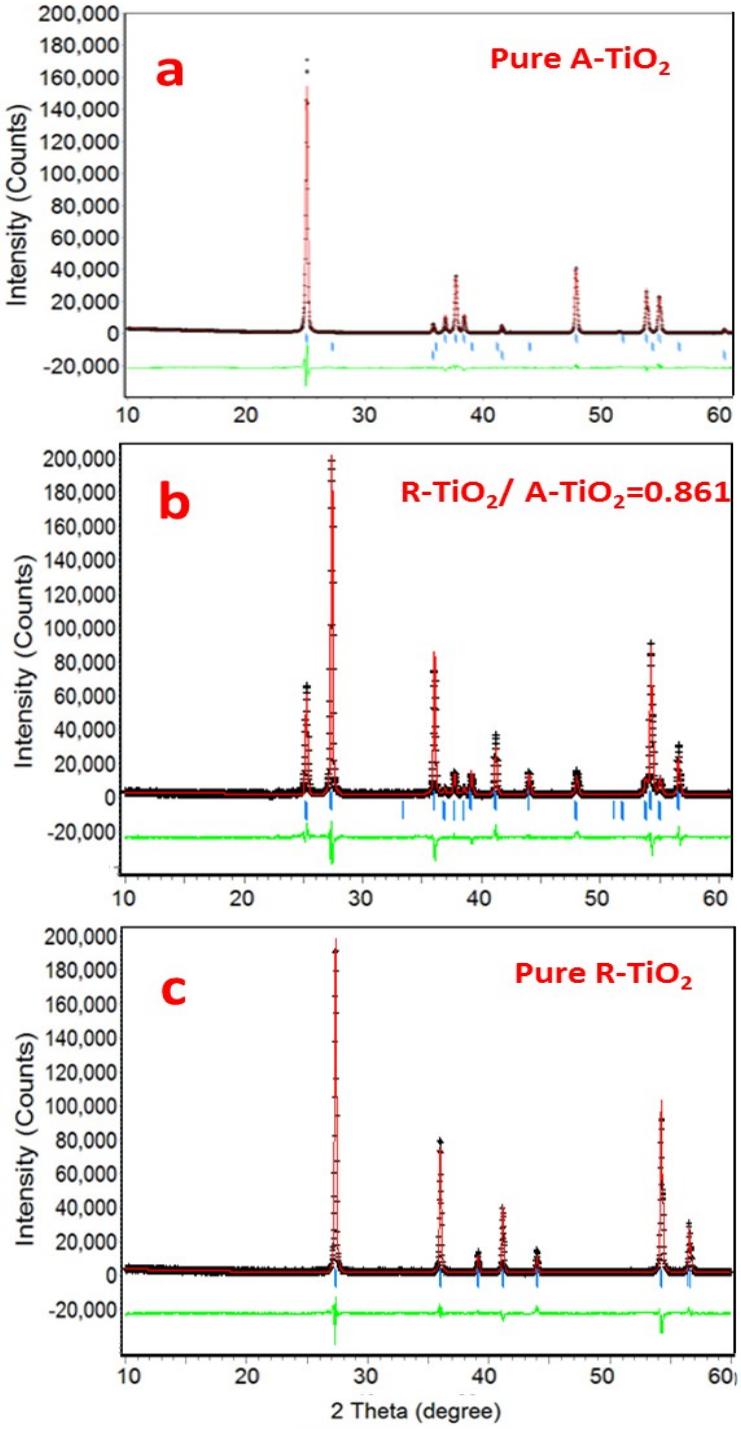

Figure S7. The typical Rietveld refinement graphs (Fullprof software) of the samples, (a) IPA+0.5EG at 300 ℃ for 24 h, (b) IPA+0.5EG+1$FeCl_3$ at 220 ℃ for 24 h. (c) IPA+0.5EG+1$FeCl_3$ at 300 ℃ for 24 h.

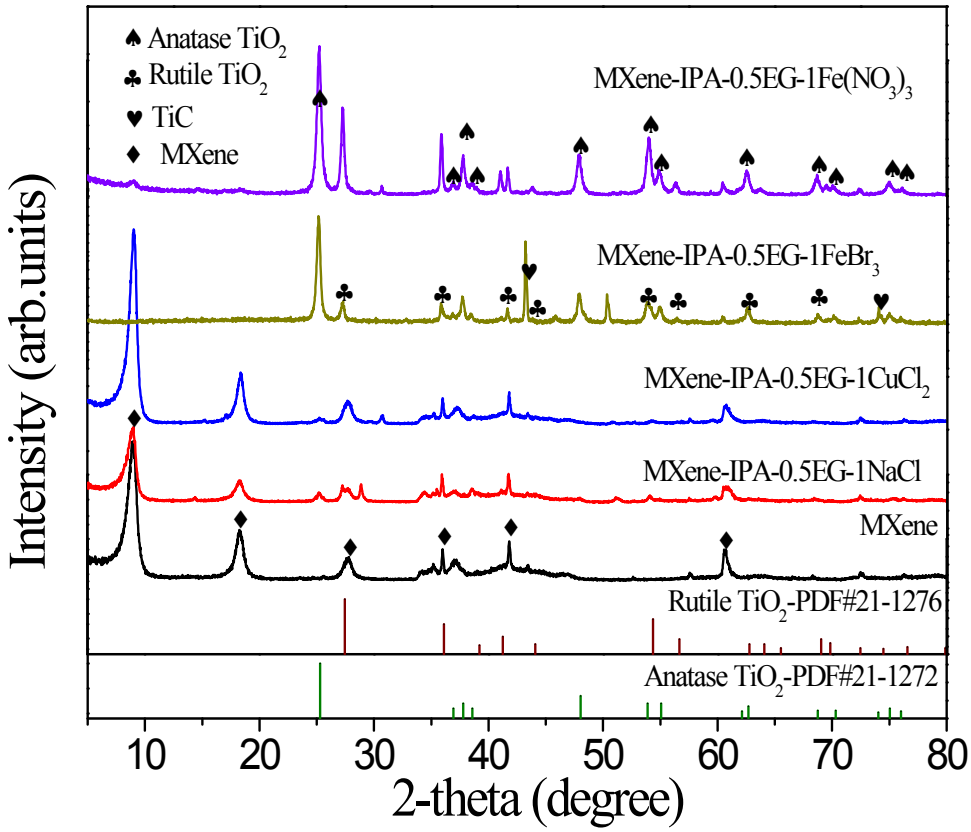

Figure S8. The effect of salts on the phase transformation of MXene at 220 ℃ for 24 h

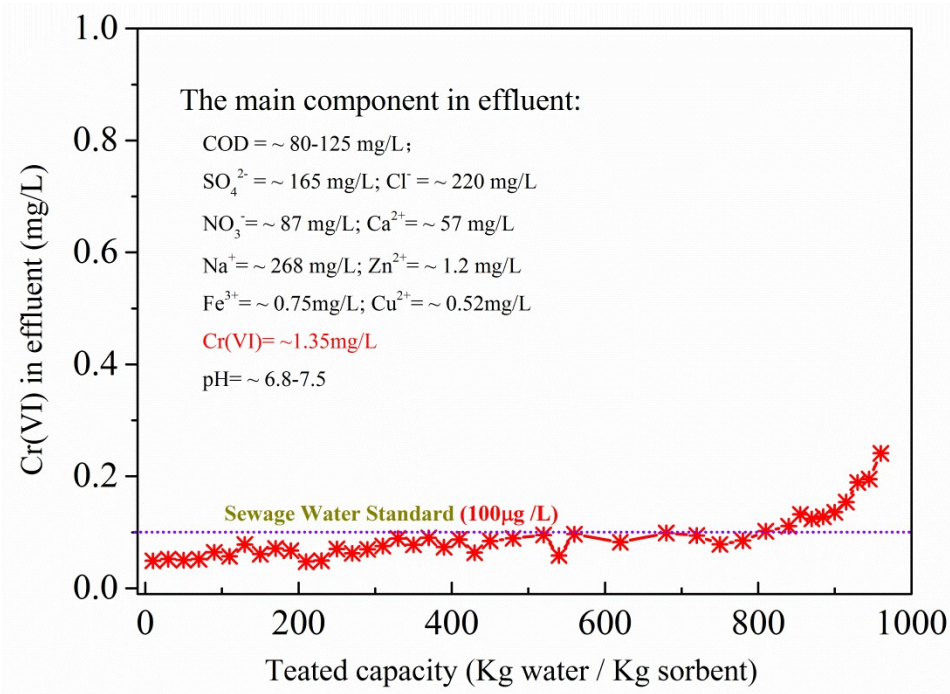

Figure S9 The real wastewater verification towards Cr(VI) removal. Note that the samples were got from the effluent of electroplating wastewater for further purification with the help of HaoYuan Environmental Engineering Co. China.

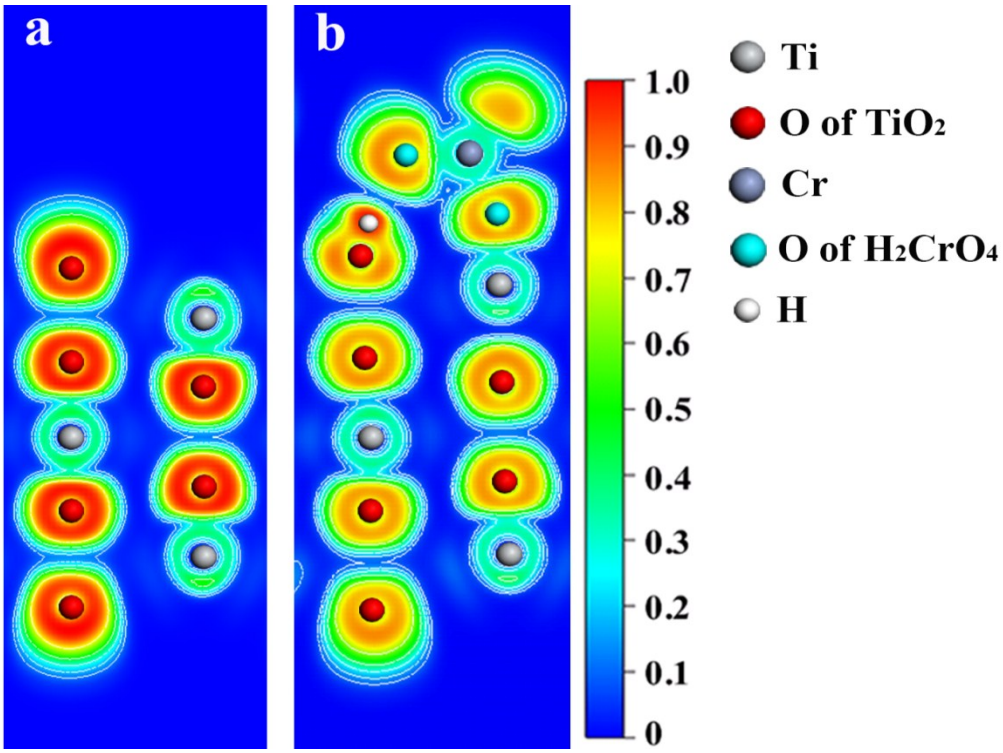

Figure S10 ELFs of R-TiO_2 (110) surface (a) and H_2CrO_4 adsorption on R-TiO_2 (110) surface (b).

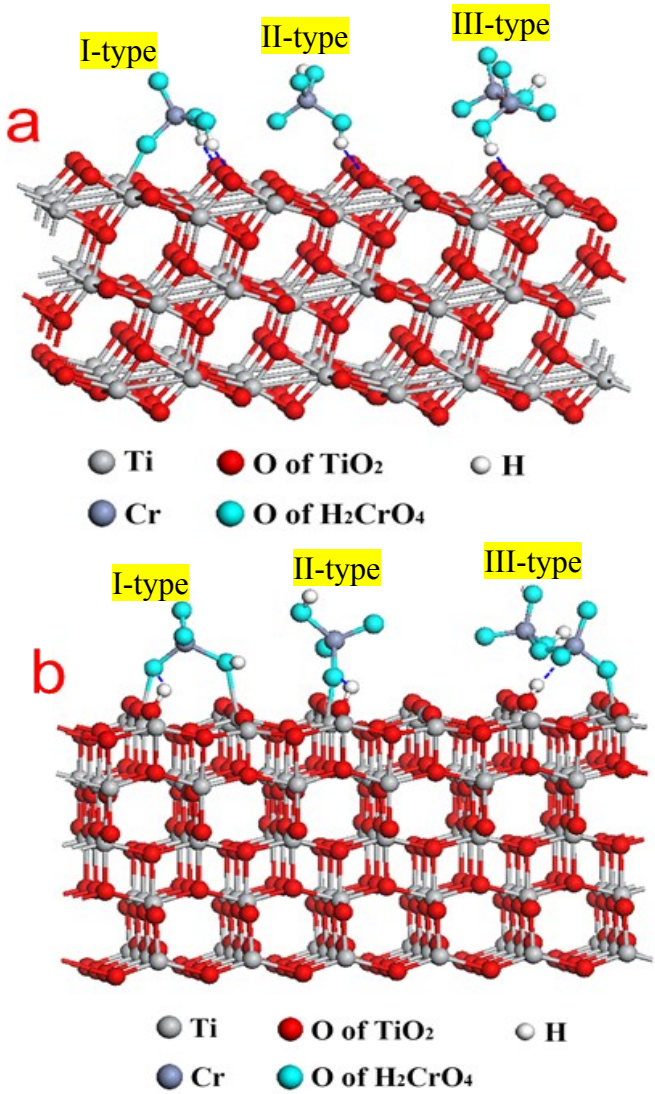

Figure S11. The adsorption sketch map of CrO_4^{2-} (I-type), $HCrO_4^-$ (II-type), and $Cr_2O_7^{2-}$ (III-type) ions using the different adsorption structures of H_2CrO_4 and $H_2Cr_2O_7$, respectively. a) A-TiO_2 (101) surface b) A-TiO_2 (001) surface.

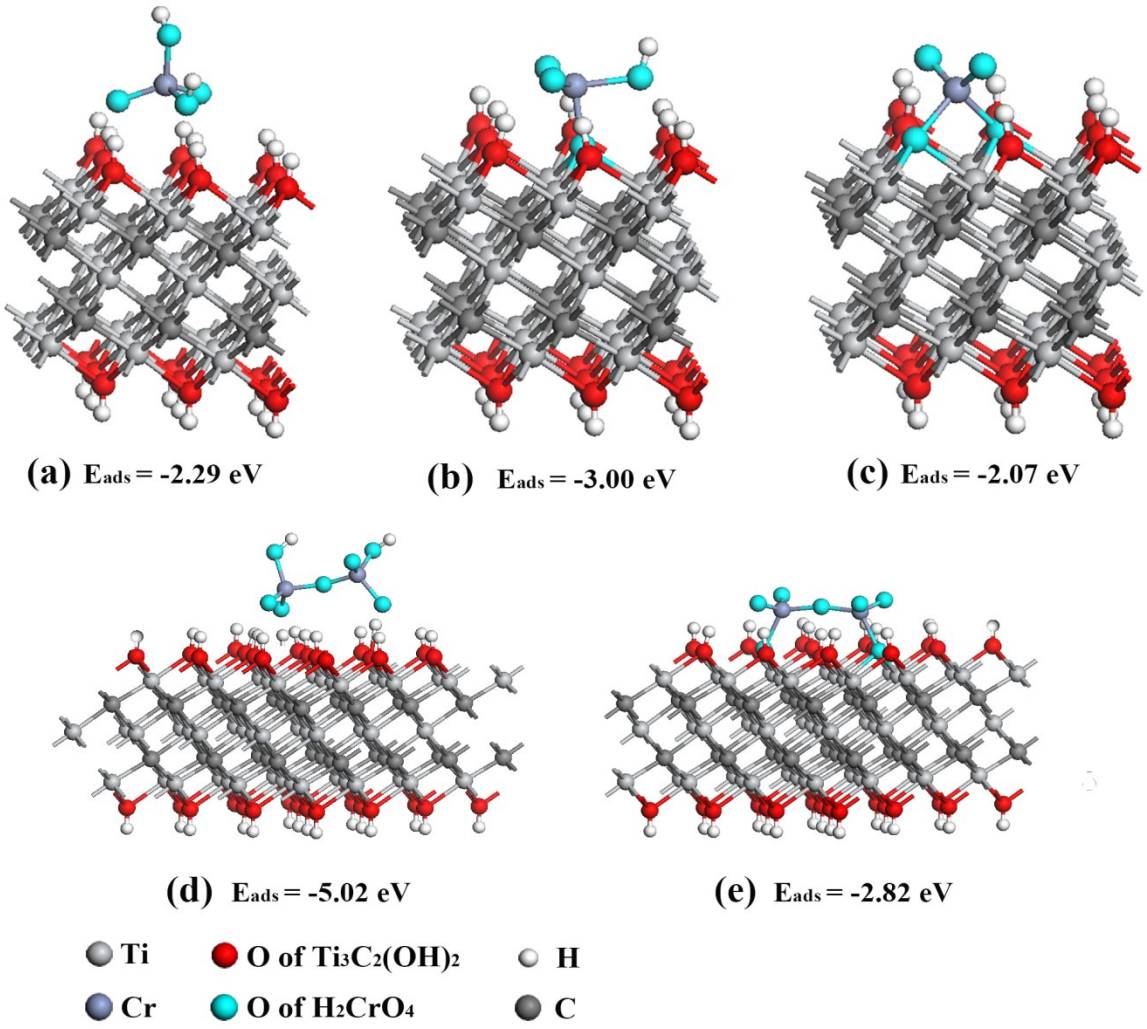

Figure S12 The sketch map and adsorption energies or formation energies of H_2CrO_4 and $H_2Cr_2O_7$ adsorption on $Ti_3C_2(OH)_2$ surface. (a) electrostatic adsorption of H_2CrO_4; the chemical adsorption by the formation of one (b) or two H_2O (c) coming from OH^- of $Ti_3C_2(OH)_2$ and H^- of H_2CrO_4; (d) electrostatic adsorption of $H_2Cr_2O_7$; (e) the chemical adsorption by the formation of one H_2O coming from OH^- of $Ti_3C_2(OH)_2$ and H^- of $H_2Cr_2O_7$.