Supplementary information

$Ti_3C_2T_x$ MXenes decorated black phosphorus nanosheets with boosted visible-light photocatalytic activity: experiment and theory studies

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Supporting Table

Table S1. Pseudo-first-order rate constants (*k*), correlation coefficients (R^2), and removal efficiency (RE) for the pollutants in different photocatalytic systems.

Samples	RhB			TCH		
	k (min^{-1})	R^2	RE (%)	*k* (min^{-1})	R^2	RE (%)
BP	0.0017	0.9681	12.75	0.0014	0.9696	9.35
TCT	0.0088	0.9966	44.08	0.0013	0.9771	10.70
TCTBP-5	0.0390	0.9806	90.94	0.0224	0.9874	74.00
TCTBP-10	0.0664	0.9984	98.25	0.0352	0.9977	88.75
TCTBP-15	0.0807	0.9742	99.09	0.0414	0.9936	92.70

Supporting Figures

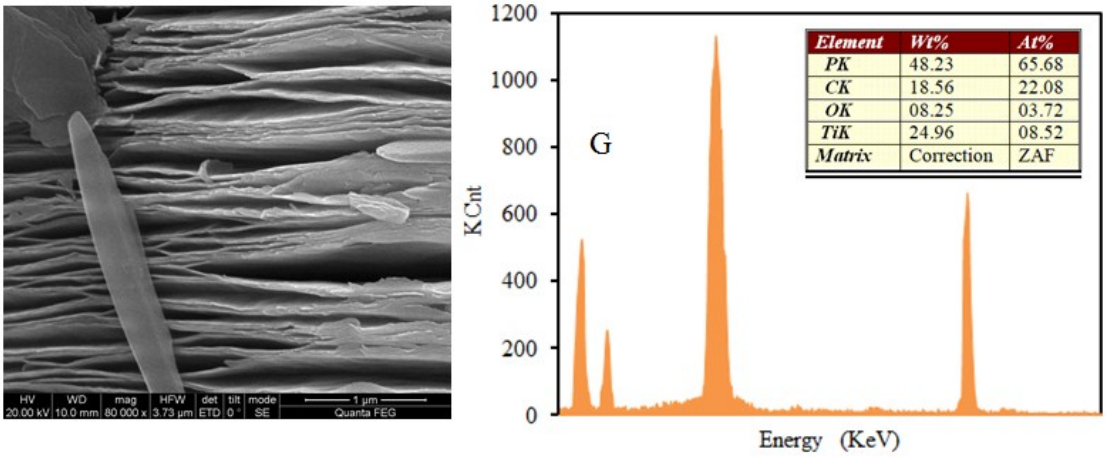

Fig. S1 SEM image of multilayered $Ti_3C_2T_x$ (left); EDS pattern of TCTBP-15 (right).

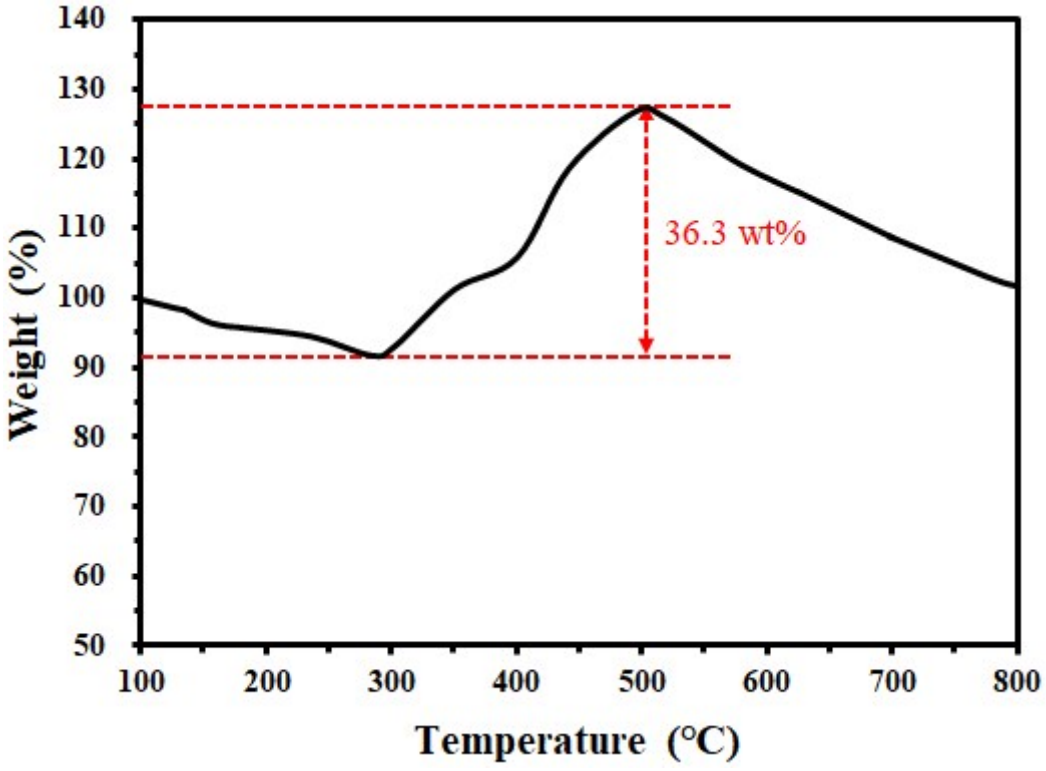

Fig. S2 TGA curve of the TiO_2/Ti_3C_2 in O_2 atmosphere.

The percent of $Ti_3C_2T_x$ and TiO_2 in $Ti_3C_2T_x/TiO_2$ was estimated by the increment of weight in thermogravimetric analysis (TGA) based on the previous studies [1, 2]. As shown in Fig. S2, there was some weight loss before 300 °C, which was ascribed to the volatilization of water on the surface and intercalated into the interlayers of the $Ti_3C_2T_x/TiO_2$. Subsequently, there was a significant mass increase (about 36.3 wt%) in TGA curve during the annealing treatment, which should be attributed to thermal oxidation of the $Ti_3C_2T_x$ at high temperature. Accordingly, the weight ratio of the $Ti_3C_2T_x$ in the resulting $Ti_3C_2T_x/TiO_2$ hybrid could be calculated to be about 84.7 wt% based on the following reaction equation: $Ti_3C_2 + 5O_2 \rightarrow 3TiO_2 + 2CO_2$. Correspondingly, the estimated proportion of TiO_2 in the $Ti_3C_2T_x/TiO_2$ hybrid was about 15.3 wt%. It should be pointed out that part of oxygen-containing or fluorine functional groups may inevitably decompose to cause a loss of weight. Therefore, the calculated TiO_2 mass (15.3 wt%) was an estimated value.

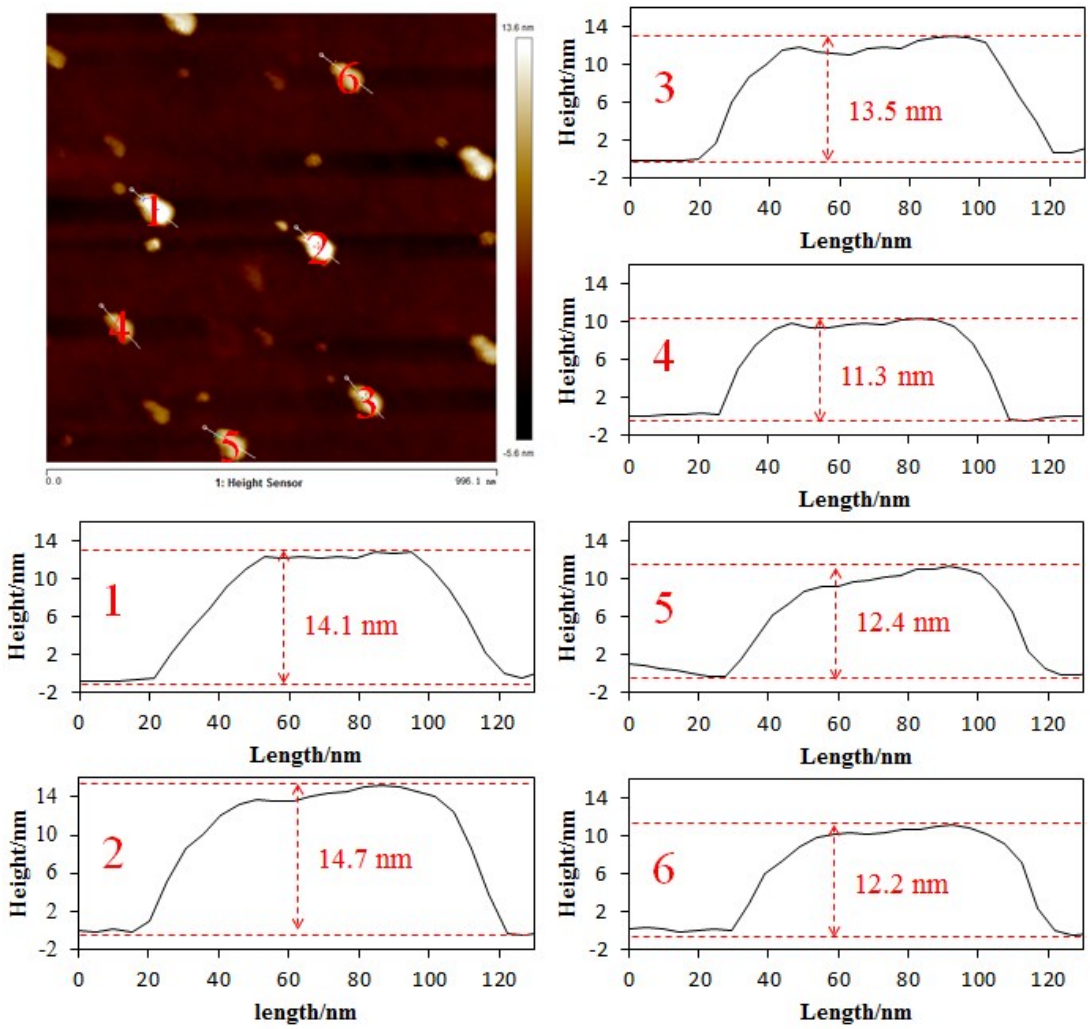

Fig. S3 AFM image and height profiles of $Ti_3C_2T_x/TiO_2$.

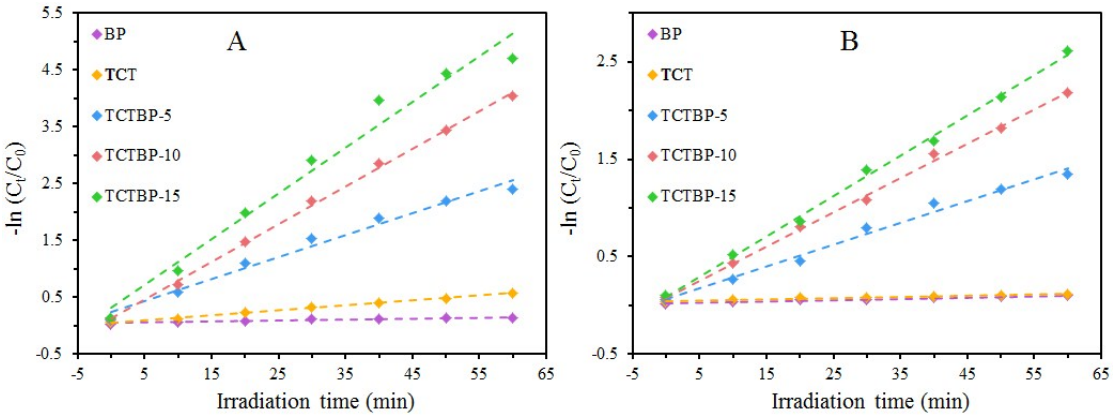

Fig. S4 The pseudo-first-order kinetic model for the photodegradation of RhB (A) and TCH (B).

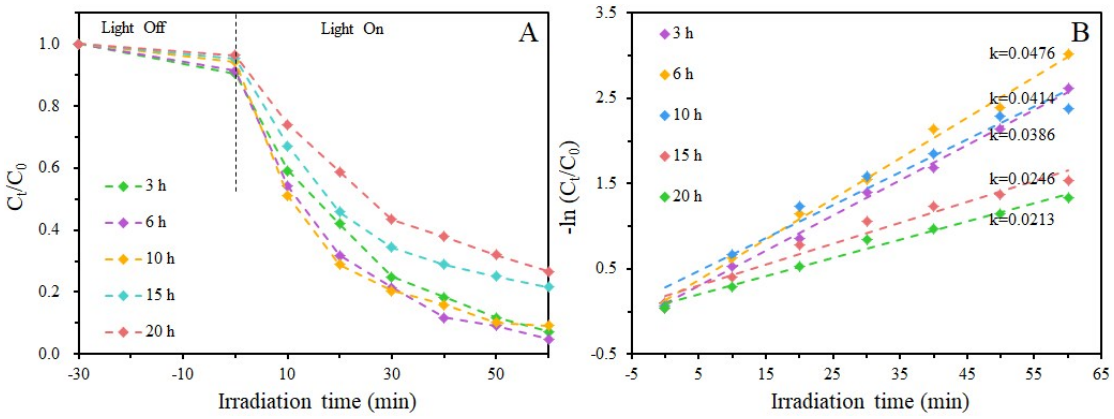

Fig. S5 The photocatalytic activities of TCTBP-15 for the photodegradation of TCH after the duration of hydrothermal treatment.

When the duration of hydrothermal treatment was too long, the photocatalytic performance for TCH degradation was reduced, which could be due to the the fraction of TiO_2 gradually increased and that of $Ti_3C_2T_x$ decreased, the previous study also reported this phenomenon [3].

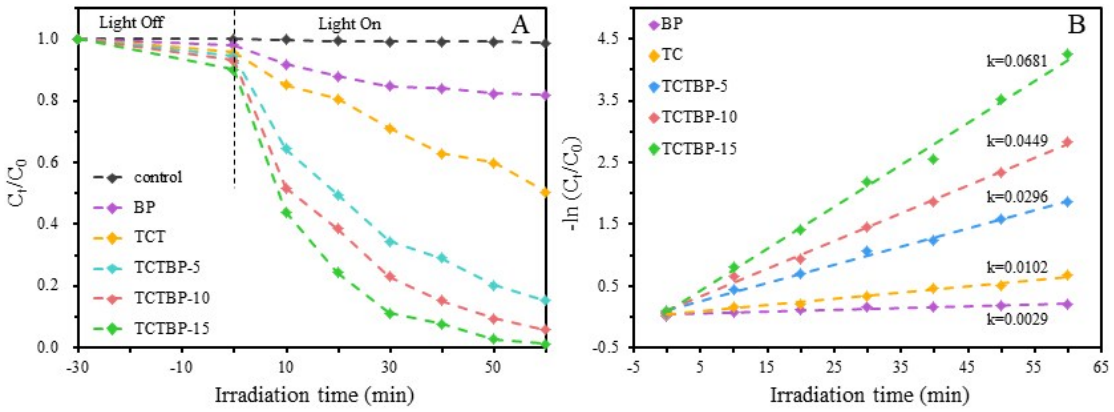

Fig. S6 The photocatalytic activities of as-prepared samples for TCH degradation under UV-Visible light illumination (the AM 1.5 optical filter has been uesd to obtain UV-Visible light).

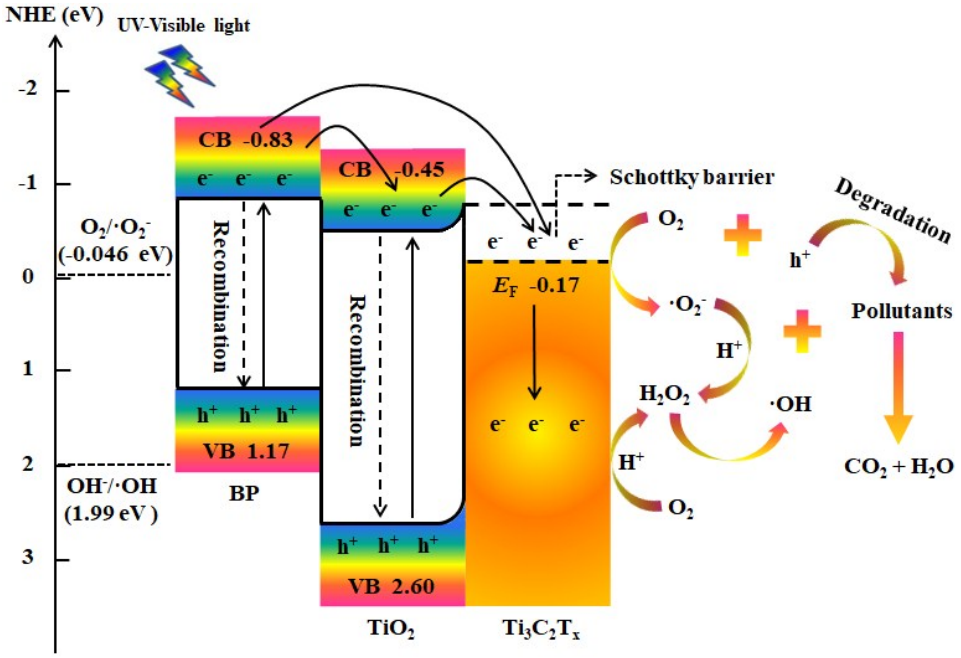

Fig. S7 Schematic diagram for possible charge separation and photocatalytic mechanism of $Ti_3C_2T_x/TiO_2$-BP composite under UV-Visible light illumination.

Obviously, the photocatalytic performance for TCH degradation has been improved in some extent, and the rate constant (*k*) was significantly increased, mewnwhile, the maximum photodegradation efficiency reached to 98.59% (for TCTBP-15). The increased photocatalytic performance could attribute to the excellent response of TiO_2 and BP to ultraviolet light, which could casue more photoinduced electrons and holes, thus accelerating the degradation of TCH.

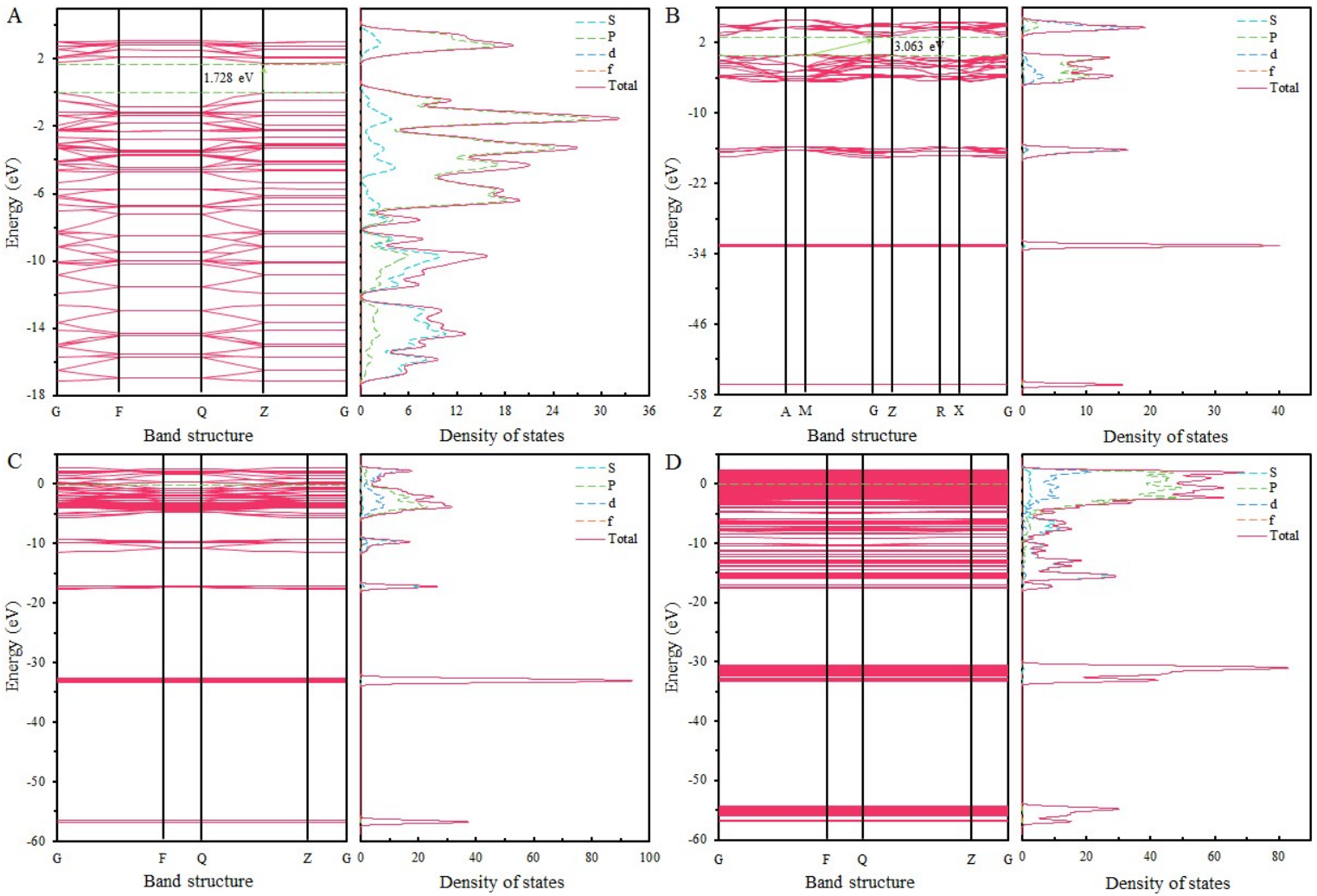

Fig. S8 Band structures and the density of states of BP (A), TiO_2 (B), $Ti_3C_2O_2$ (C) and $Ti_3C_2O_2/TiO_2$-BP (D).

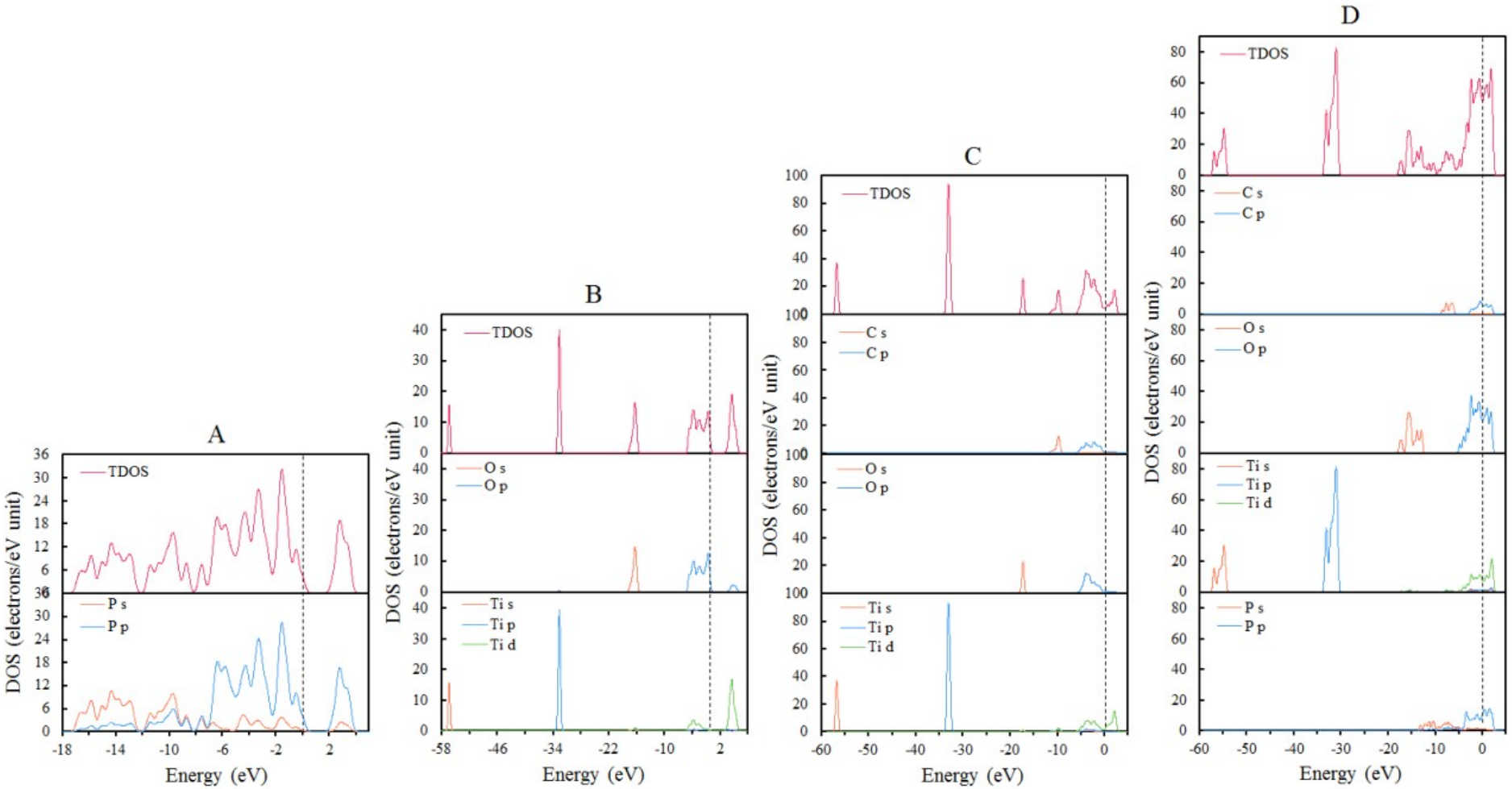

Fig. S9 TDOS and PDOS of BP (A), TiO_2 (B), $Ti_3C_2O_2$ (C) and $Ti_3C_2O_2/TiO_2$-BP (D).

References

1. T. Xu, J. Wang, Y. Cong, S. Jiang, Q. Zhang, H. Zhu, Y. Li and X. Li, *Chinese Chemical Letters*, 2019.
2. C. Yang, Y. Liu, X. Sun, Y. Zhang, L. Hou, Q. Zhang and C. Yuan, *Electrochimica Acta*, 2018, **271**, 165-172.
3. C. Peng, X. Yang, Y. Li, H. Yu, H. Wang and F. Peng, *ACS Applied Materials & Interfaces*, 2016, **8**, 6051-6060.