

Supplementary Information

for

Synergistic Effects of Nonmetals Co-doping with Sulfur in Anatase TiO₂: A

DFT+U Study

Qing-Lu Liu^{1,3}, Zong-Yan Zhao^{2,*}, Qing-Ju Liu^{3,*}

¹ School of Physical Science and Technology, Yunnan University, Kunming 650091, People's Republic of China

² Faculty of Materials Science and Engineering, Key Laboratory of Advanced Materials of Yunnan Province, Kunming University of Science and Technology, Kunming 650093, People's Republic of China

³ Yunnan Key Laboratory of Micro/Nano Materials & Technology, Research Institute of Engineering and Technology, Yunnan University, Kunming 650091, People's Republic of China

* Corresponding authors: zzy@kmust.edu.cn (Z. Zhao); qjliu@ynu.edu.cn (Q. Liu)

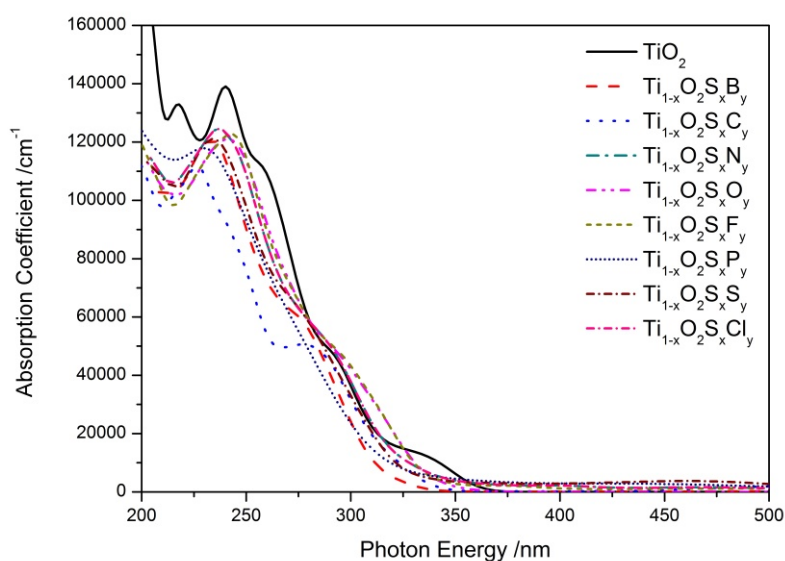


Fig. S1 Calculated absorption curves of pure TiO₂ and Ti_{1-x}O₂S_xNM_y (NM=B, C, N, O, F, P, S and Cl).

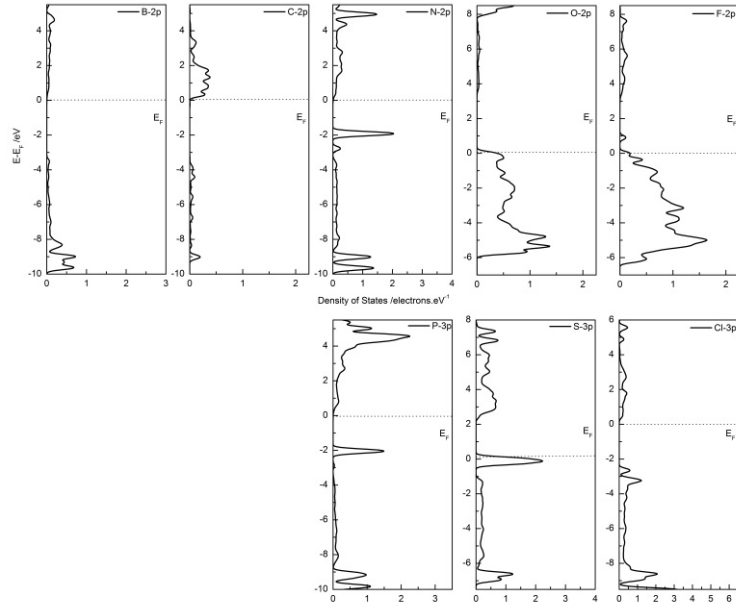


Fig. S2 Calculated partial density of states of NM- np states in $Ti_{1-x}O_2S_xNM_y$ (NM=B, C, N, O, F, P, S and Cl).

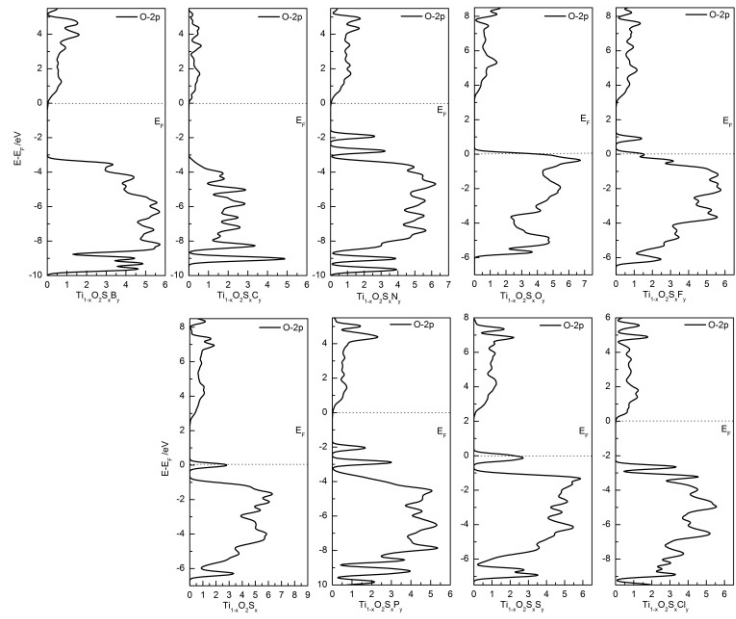


Fig. S3 Calculated partial density of states of O- $2p$ states neighboring with S_s impurity in $Ti_{1-x}O_2S_xNM_y$ (NM=B, C, N, O, F, P, S and Cl).

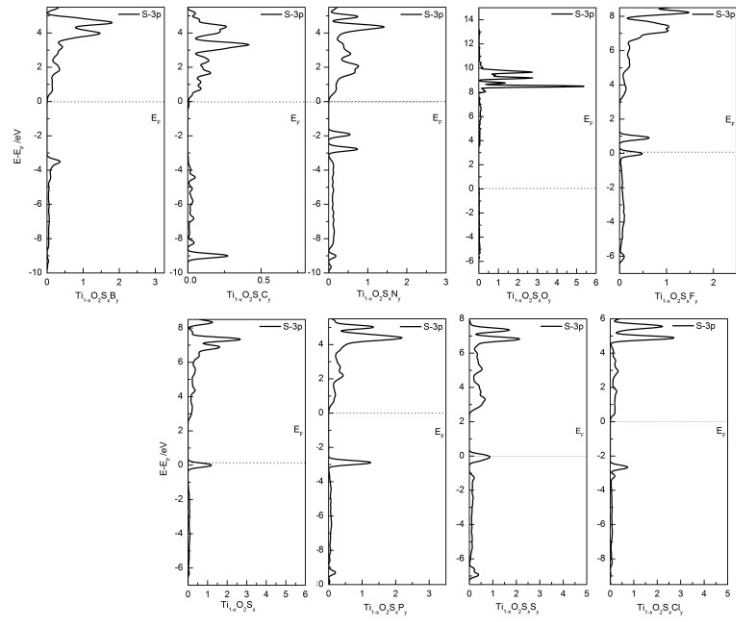


Fig. S4 Calculated partial density of states of S_s -3p states in $Ti_{1-x}O_2S_xNM_y$ (NM=B, C, N, O, F, P, S and Cl).