Supplementary Information

for

Synergistic Effects of Nonmetals Co-doping with Sulfur in Anatase TiO$_2$: A DFT+U Study

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Fig. S1 Calculated absorption curves of pure TiO$_2$ and Ti$_{1-x}$O$_2$S$_x$NM$_y$ (NM=B, C, N, O, F, P, S and Cl).

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Fig. S2 Calculated partial density of states of NM-np states in Ti$_{1-x}$O$_2$S$_x$NM$_y$ (NM=B, C, N, O, F, P, S and Cl).

Fig. S3 Calculated partial density of states of O-2p states neighboring with S$_x$ impurity in Ti$_{1-x}$O$_2$S$_x$NM$_y$ (NM=B, C, N, O, F, P, S and Cl).
Fig. S4 Calculated partial density of states of S-$\varepsilon$-3p states in Ti$_{1-x}$O$_2$S$_x$NM$_y$ (NM=B, C, N, O, F, P, S and Cl).