# *Supporting Information*

## Promoting superoxide generation in $Bi_2WO_6$ by less electronegative substitution for enhanced photocatalytic performance: an example of Te doping

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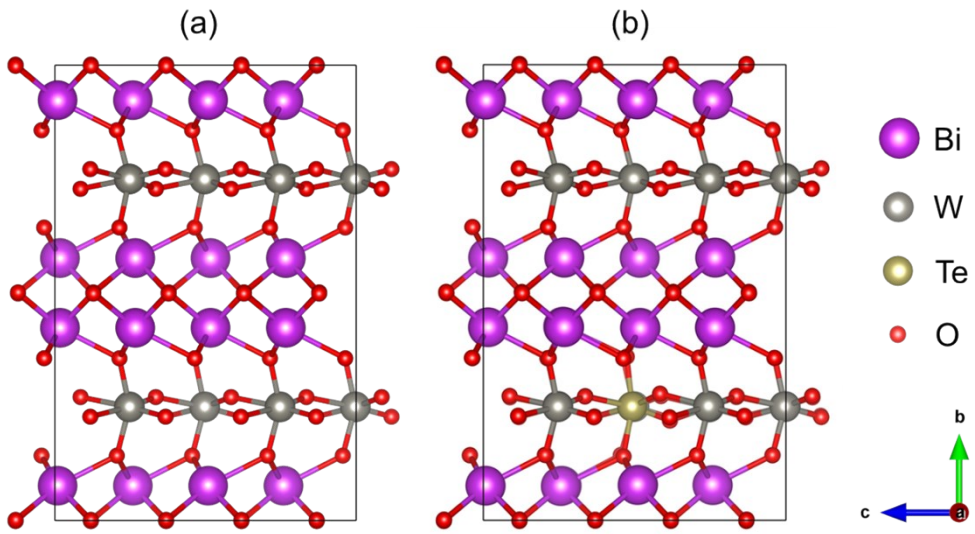


**Fig. S1** Crystal structure of $Bi_2WO_6$ (a) and Te-$Bi_2WO_6$ (b)

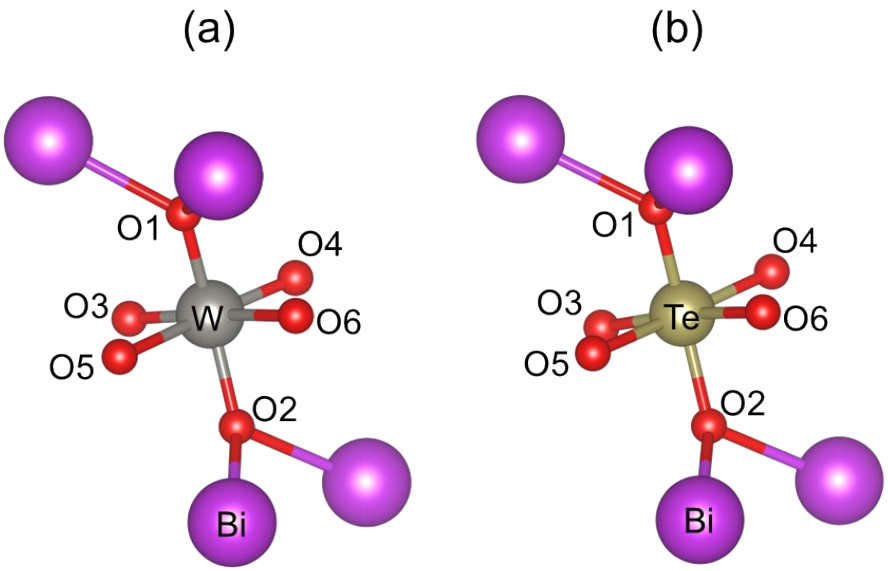


**Fig. S2** Local structures of $Bi_2WO_6$ (a) and Te-$Bi_2WO_6$ (b).

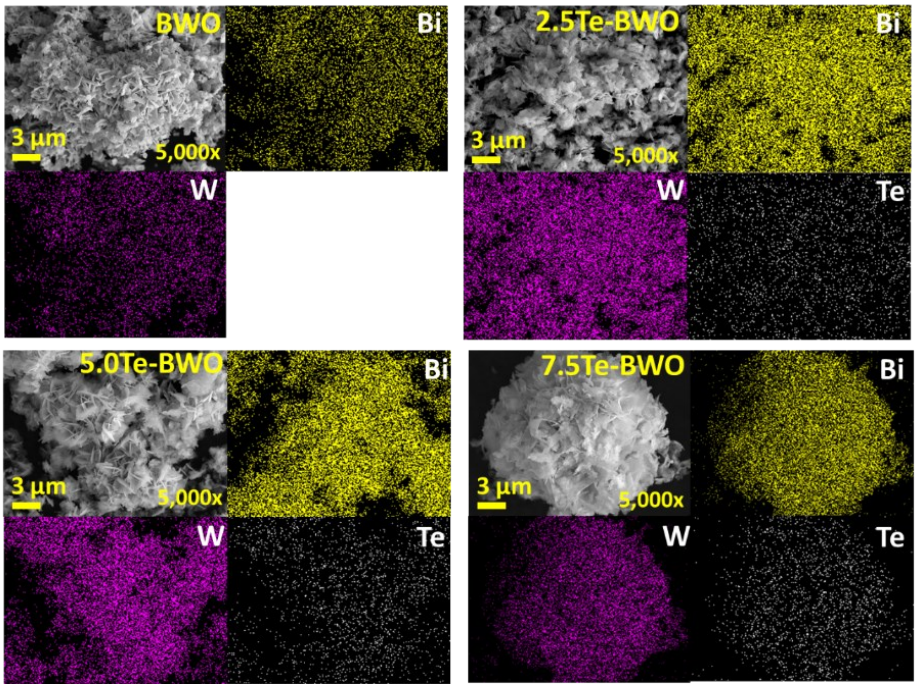


**Fig. S3** EDS mapping of BWO, 2.5Te-BWO, 5.0Te-BWO, and 7.5Te-BWO

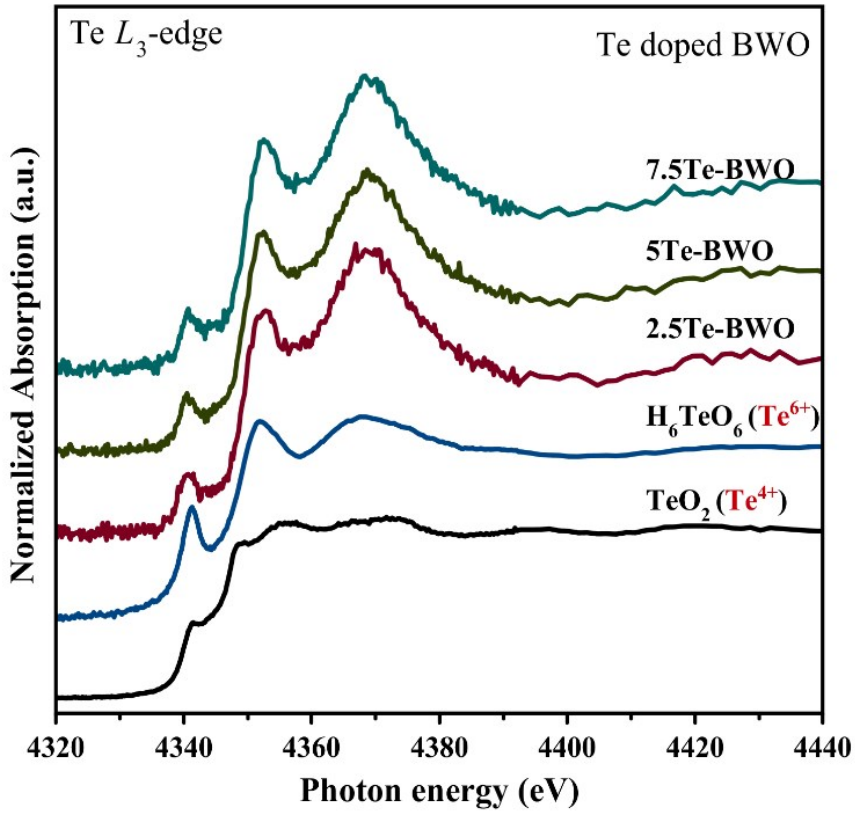


**Fig. S4** Te $L_3$-edge X-ray absorption near-edge structure (XANES) of BWO, 2.5Te-BWO, 5.0Te-BWO, and 7.5Te-BWO.

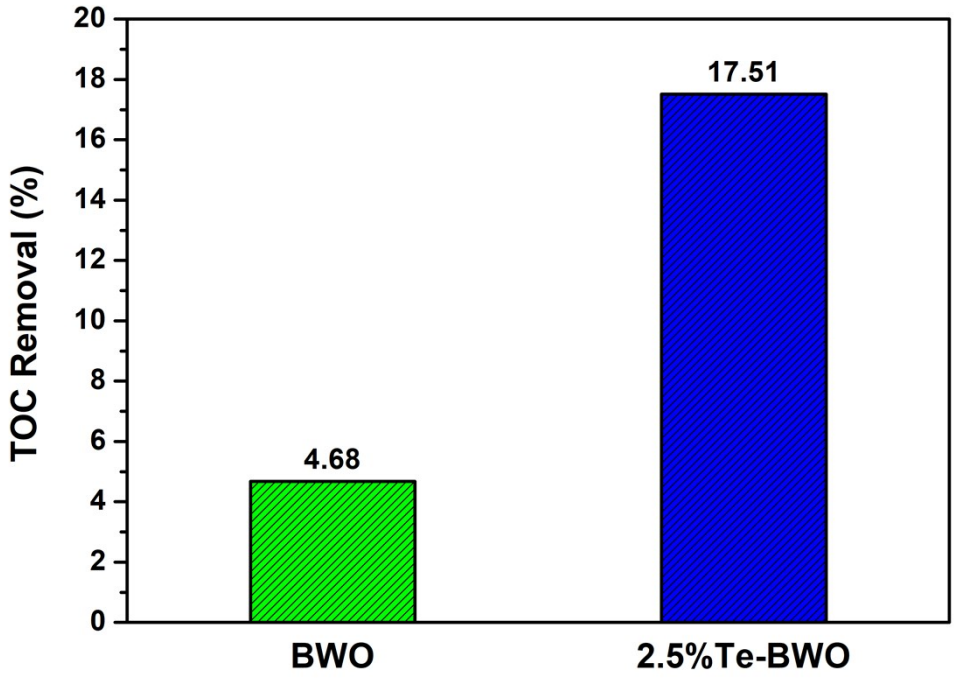


**Fig. S5** The corresponding TOC removal under visible light after 180 min of BWO, 2.5Te-BWO.

**Table S1** Calculated bond distances of pristine and Te-doped $Bi_2WO_6$. Their structures are shown in Fig. S2.

| Bond | Bond distance (Å) | |
|---|---|---|
| | $Bi_2WO_6$ | Te-doped $Bi_2WO_6$ |
| W(Te)–O1 | 1.882 | 1.895 |
| W(Te)–O2 | 1.886 | 1.898 |
| W(Te)–O3 | 1.810 | 1.909 |
| W(Te)–O4 | 1.818 | 1.918 |
| W(Te)–O5 | 2.206 | 2.129 |
| W(Te)–O6 | 2.191 | 2.115 |

**Table S2** Bader charge in pristine and Te-doped $Bi_2WO_6$. The positive and negative values represent the depletion and accumulation of electrons, respectively. The corresponding structures are shown in Fig. S2.

| Atom | Bader charge (e) | |
|---|---|---|
| | $Bi_2WO_6$ | Te-doped $Bi_2WO_6$ |
| W(Te) | +2.62 | +2.98 |
| O1 | −1.06 | −1.11 |
| O2 | −1.07 | −1.11 |
| O3 | −0.98 | −1.14 |
| O4 | −0.99 | −1.14 |
| O5 | −0.98 | −1.01 |
| O6 | −0.99 | −1.03 |

**Table S3**. List of the band edge potential of various ions doped $Bi_2WO_6$ and oxygen vacancy with base on experiment.

| Sample | Eg (eV) | $E_{VB}$ *vs.* NHE (eV) | $EC_B$ *vs.* NHE (eV) | EN value[1-3] | Ref |
|---|---|---|---|---|---|
| $Bi_2WO_6$ | 2.94 | 1.84 | -0.93 | | |
| 3%Ti-$Bi_2WO_6$ | 2.85 | 1.99 | -1.06 | 1.54 (Ti) | [4] |
| $Bi_2WO_6$ | 2.71 | 2.28 | -0.33 | | |
| 10%Ti- $Bi_2WO_6$ | 2.84 | 2.33 | -0.41 | 1.54 (Ti) | [5] |
| $Bi_2WO_6$ | 3.00 | 2.98 | -0.02 | | |
| 0.26%Fe- $Bi_2WO_6$ | ~2.97 | 2.77 | -0.20 | 1.83 (Fe) | [6] |
| $Bi_2WO_6$ | 2.96 | 3.18 | 0.22 | | |
| 21%Mo- $Bi_2WO_6$ | 2.43 | 2.50 | 0.05 | 2.16 (Mo) | [7] |
| $Bi_2WO_6$ | 2.62 | 3.38 | 0.76 | | |
| 4%P- $Bi_2WO_6$ | 2.71 | 3.43 | 0.72 | 2.19 (P) | [8] |
| $Bi_2WO_6$ | 2.93 | 1.60 | -1.33 | | |
| $Bi_2WO_{6-x}$ | 2.75 | 1.28 | -1.57 | 3.44 (O) | [9] |

The electronegativities of Bi, W, and O are 2.02, 2.36, and 3.44, respectively[1-3]

## References


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