

SUPPORTING INFORMATION

Near-Infrared Photocatalytic Activity Induced by Intrinsic Defects in Bi_2MO_6

($\text{M}=\text{W}, \text{Mo}$)

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Figure S1 Energy band of (a) $\text{Bi}_{\text{vac}}\text{-Bi}_2\text{WO}_6$, (b) $\text{W}_{\text{vac}}\text{-Bi}_2\text{WO}_6$, (c) $\text{Bi}_{\text{W}}\text{-Bi}_2\text{WO}_6$, (d) $\text{W}_{\text{Bi}}\text{-Bi}_2\text{WO}_6$, (e) $\text{W}_{\text{int}}\text{-Bi}_2\text{WO}_6$, (f) $\text{O}_{\text{int}}\text{-Bi}_2\text{WO}_6$. The red dashed lines represent the Fermi level, which is set to zero.

Figure S2 Projected density of states (PDOS) of (a) $\text{Bi}_{\text{vac}}\text{-Bi}_2\text{WO}_6$, (b) $\text{W}_{\text{vac}}\text{-Bi}_2\text{WO}_6$, (c) $\text{Bi}_{\text{W}}\text{-Bi}_2\text{WO}_6$, (d) $\text{W}_{\text{Bi}}\text{-Bi}_2\text{WO}_6$, (e) $\text{W}_{\text{int}}\text{-Bi}_2\text{WO}_6$, (f) $\text{O}_{\text{int}}\text{-Bi}_2\text{WO}_6$.

Figure S3 Energy band of (a) $\text{Bi}_{\text{vac}}\text{-Bi}_2\text{MoO}_6$, (b) $\text{Mo}_{\text{vac}}\text{-Bi}_2\text{MoO}_6$, (c) $\text{Bi}_{\text{Mo}}\text{-Bi}_2\text{MoO}_6$, (d) $\text{Mo}_{\text{Bi}}\text{-Bi}_2\text{MoO}_6$, (e) $\text{Mo}_{\text{int}}\text{-Bi}_2\text{MoO}_6$, (f) $\text{O}_{\text{int}}\text{-Bi}_2\text{MoO}_6$. The red dashed lines represent the Fermi level, which is set to zero.

Figure S4 Projected density of states (PDOS) of (a) $\text{Bi}_{\text{vac}}\text{-Bi}_2\text{MoO}_6$, (b) $\text{Mo}_{\text{vac}}\text{-Bi}_2\text{MoO}_6$, (c) $\text{Bi}_{\text{Mo}}\text{-Bi}_2\text{MoO}_6$, (d) $\text{Mo}_{\text{Bi}}\text{-Bi}_2\text{MoO}_6$, (e) $\text{Mo}_{\text{int}}\text{-Bi}_2\text{MoO}_6$, (f) $\text{O}_{\text{int}}\text{-Bi}_2\text{MoO}_6$.

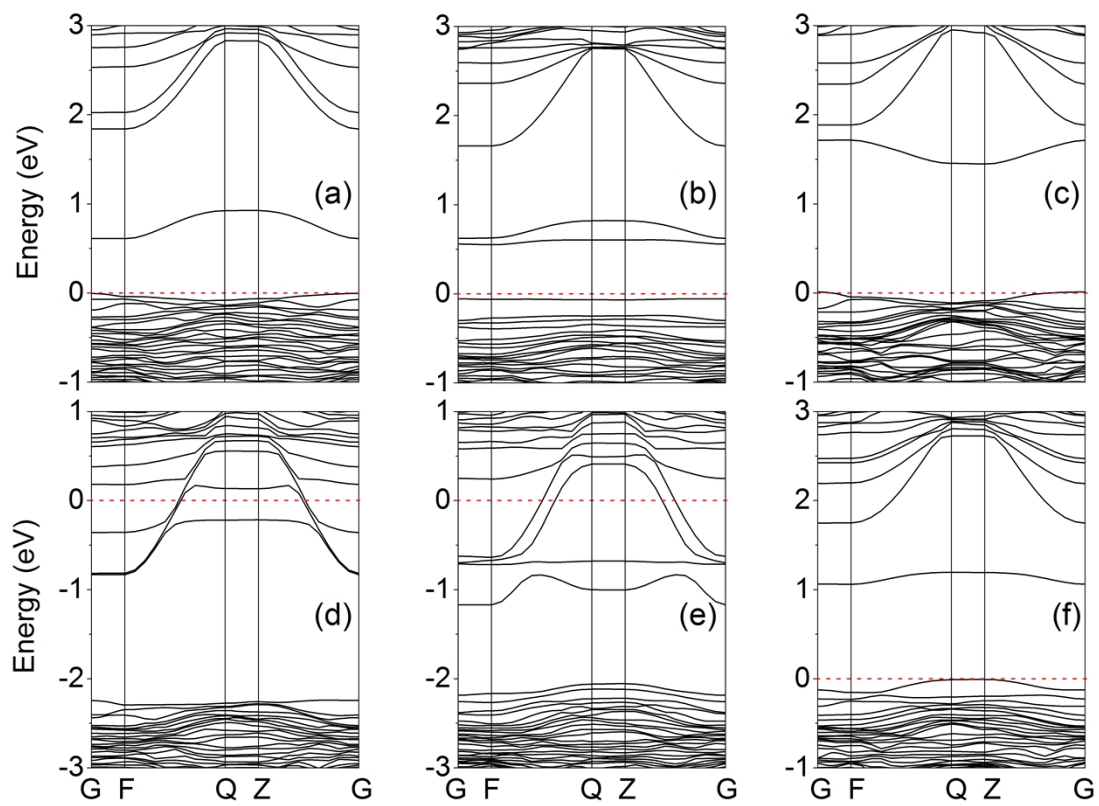


Figure S1

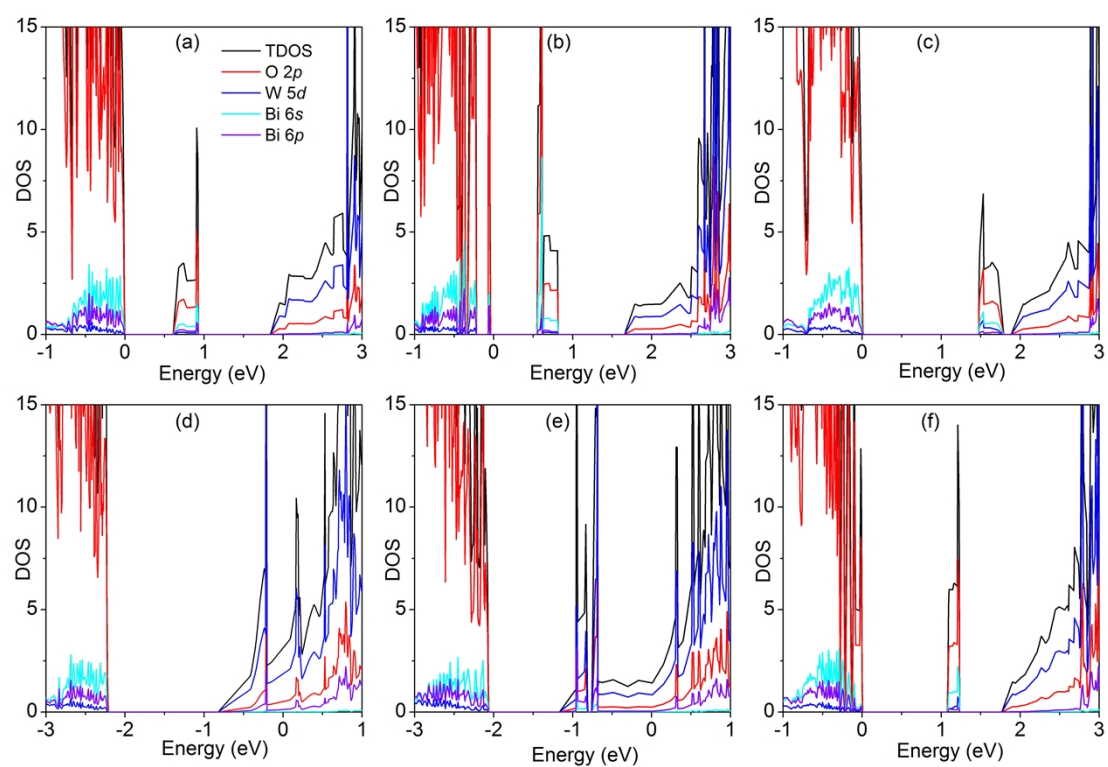


Figure S2

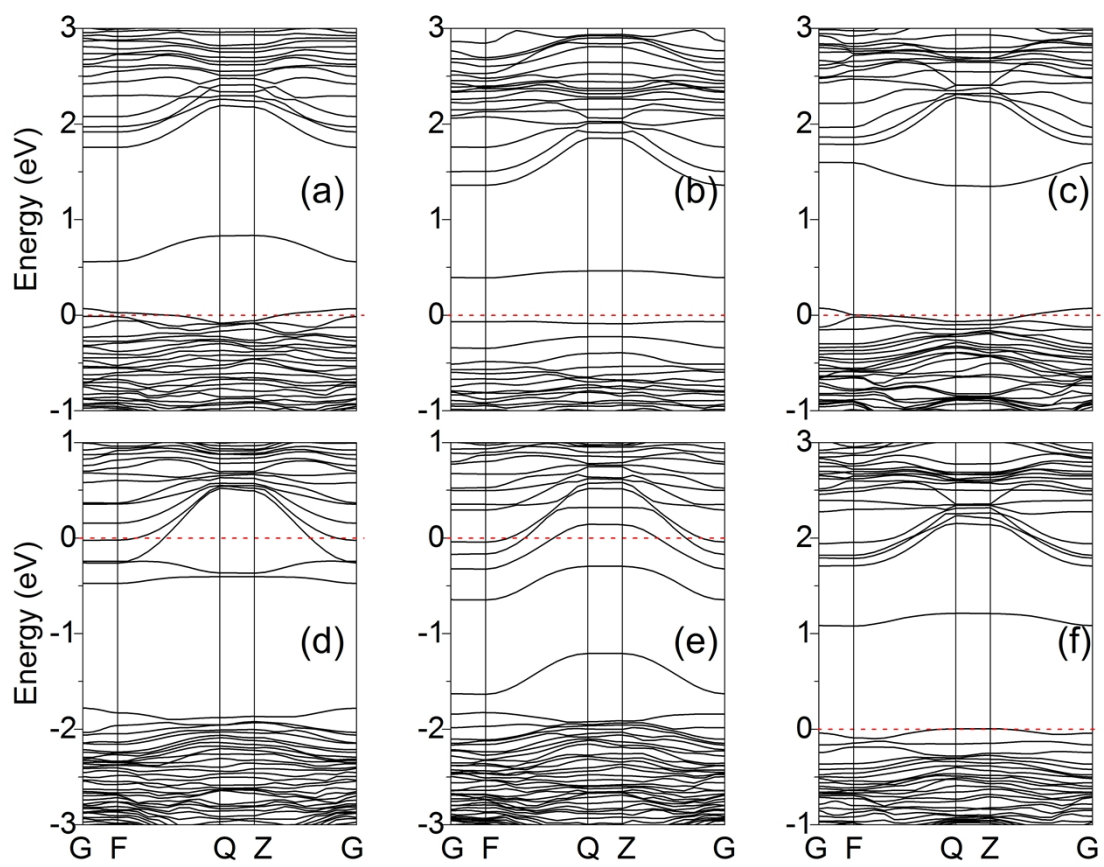


Figure S3

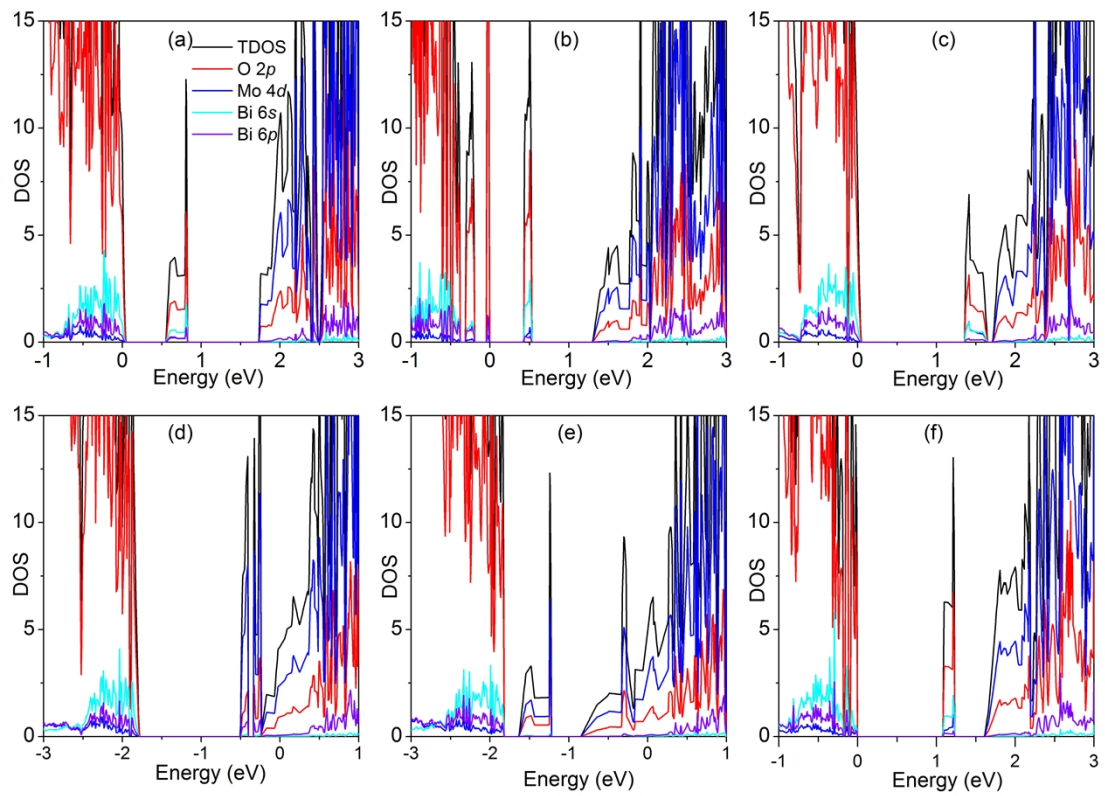


Figure S4