

Supplementary Materials for

**Enhanced photocatalytic activities of Bi_2WO_6 by introducing Zn
to replace Bi lattice sites: a first-principles study**

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I. FIGURE CAPTIONS

Fig. S1. The projected density of state (PDOS) (a) and band structure (b) of $\text{Bi}_{1.875}\text{Zn}_{0.125}\text{WO}_6$.

Fig. S2. The projected density of state (PDOS) (a) and band structure (b) of $\text{Bi}_{1.5}\text{Zn}_{0.5}\text{WO}_6$.

Fig. S3. The projected density of state (PDOS) (a) and band structure (b) of $\text{Bi}_{1.75}\text{Cd}_{0.25}\text{WO}_6$.

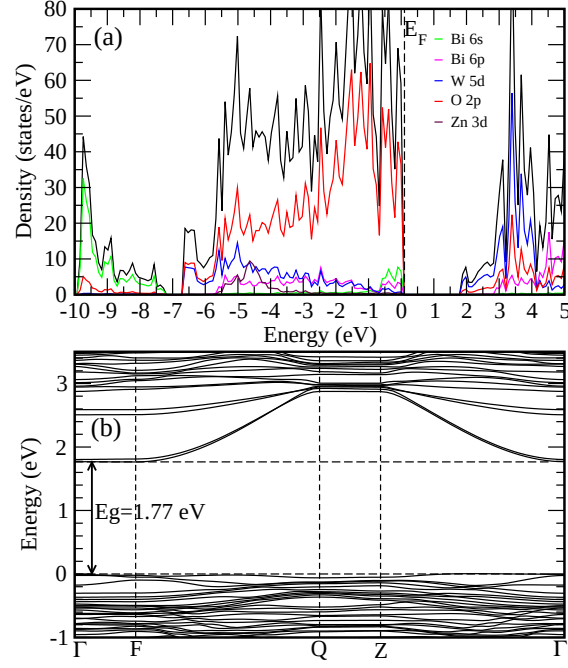


FIG. 1: The projected density of state (PDOS) (a) and band structure (b) of Bi_{1.875}Zn_{0.125}WO₆.

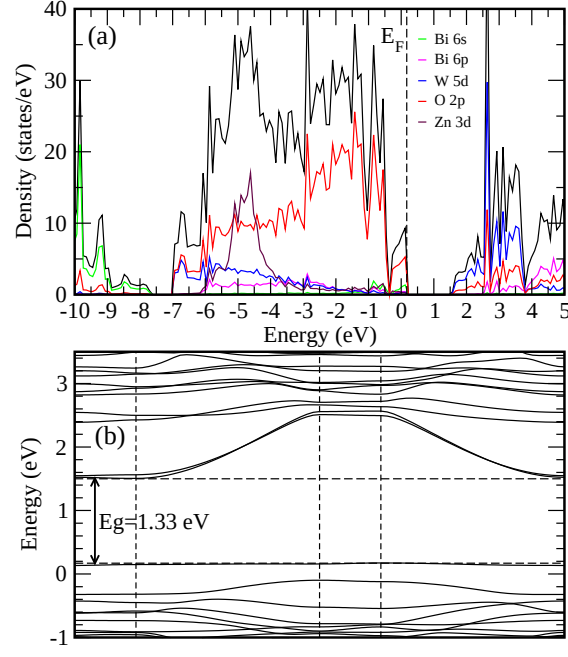


FIG. 2: The projected density of state (PDOS) (a) and band structure (b) of $\text{Bi}_{1.5}\text{Zn}_{0.5}\text{WO}_6$.

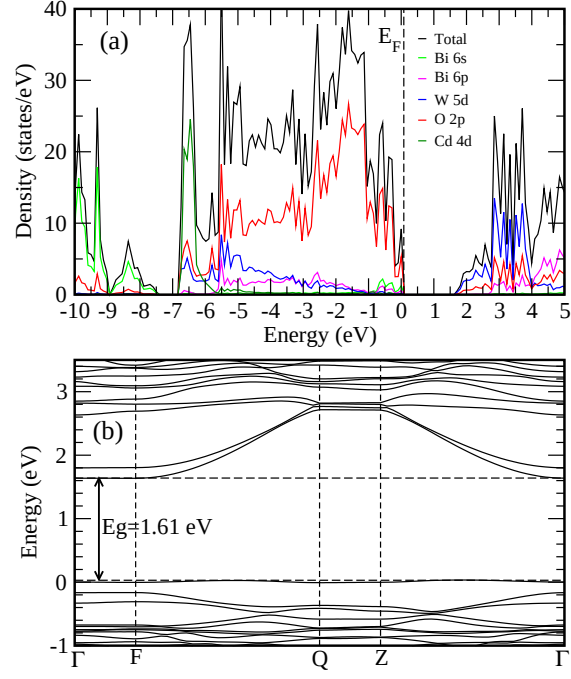


FIG. 3: The projected density of state (PDOS) (a) and band structure (b) of Bi_{1.75}Cd_{0.25}WO₆.