Supporting Information

Effects of Mo/W codoping on the visible-light photocatalytic activity of monoclinic BiVO4 within the GGA+ U framework

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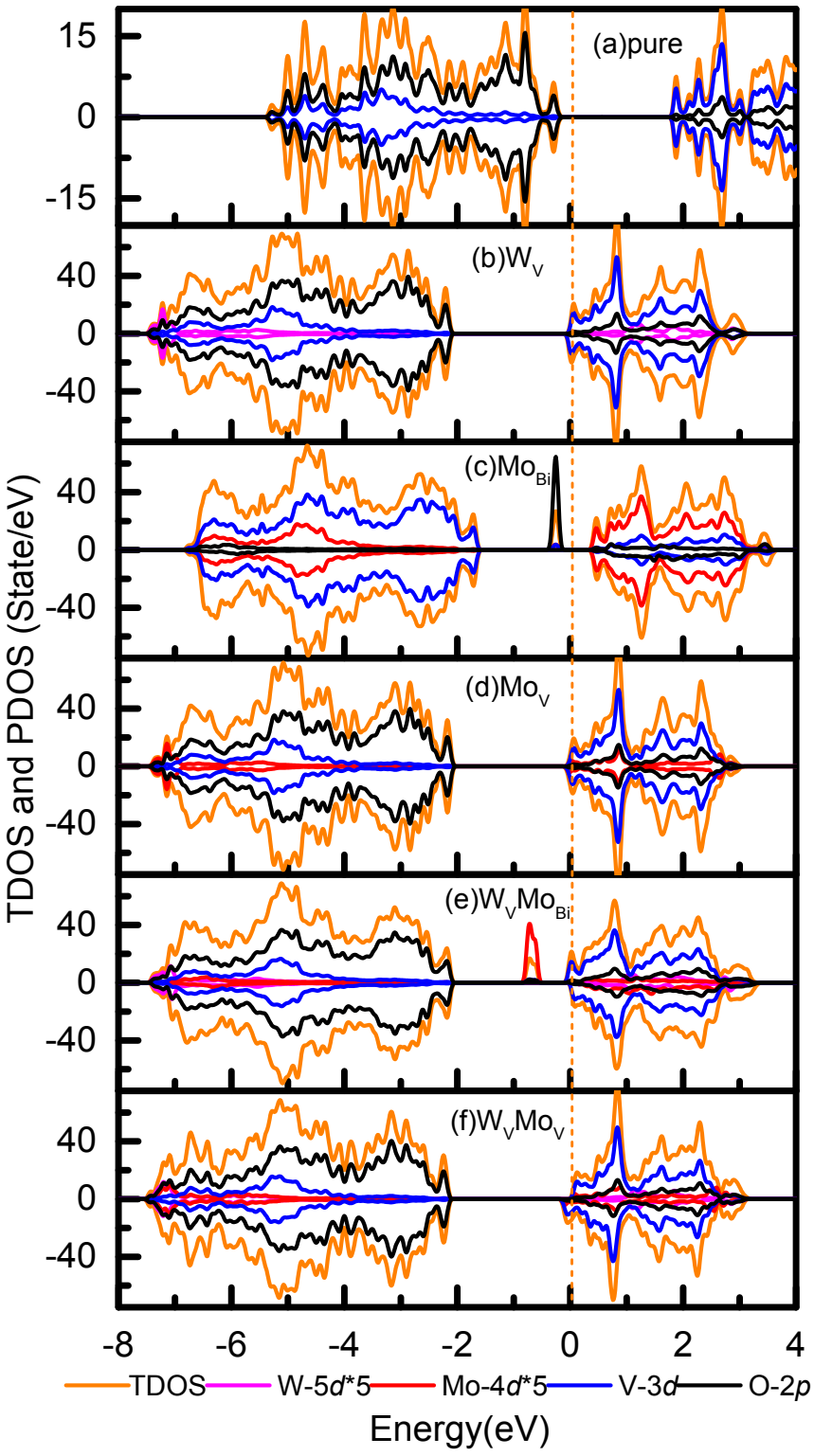

Fig. S1 DOS of pure, Mo,W mono-doped and Mo/W cod-oped $BiVO_4$: (a)pure, (b)W_V, (c)Mo_{Bi}, (d)Mo_V, (e) W_VMo_{Bi} (f) W_VMo_V, from DFT calculations. The dashed lines stand for the Fermi level (at 0eV). The orange lines represent the total DOS (TDOS) black for O 2*p*, blue for V 3*d*, red for the quadruplicate of Mo 4*d* and magenta for the quadruplicate of W 5*d*, respectively. The Mo 4d and W 5d states are multiplied by 4 times to show their distribution clearly. The dashed lines stand for the Fermi level (at 0eV).

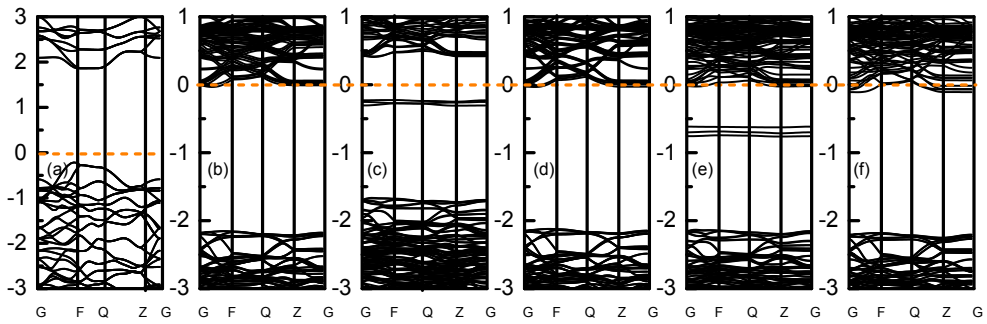

Fig. S2 Band structures of pure, Mo,W mono-doped and Mo/W co-doped $BiVO_4$: (a)pure, (b)W_V, (c)Mo_{Bi}, (d)Mo_V, (e) W_VMo_{Bi} (f) W_VMo_V, from DFT(GGA) calculations. The dashed lines stand for the Fermi level (at 0eV).

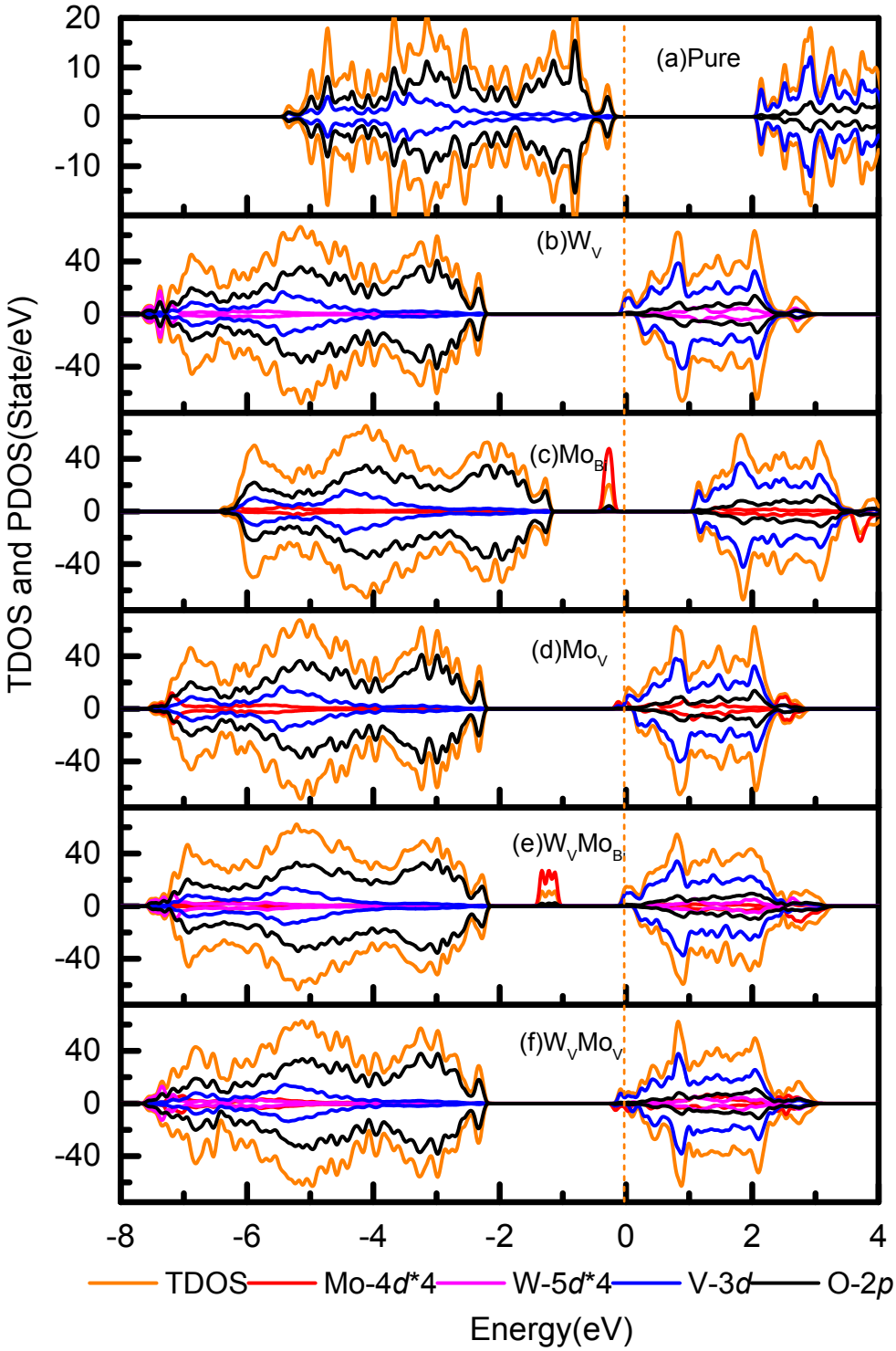

Fig. S3 DOS of pure, Mo,W mono-doped and Mo/W co-doped $BiVO_4$: (a)pure, (b)W_V, (c)Mo_{Bi}, (d)Mo_V, (e) W_VMo_{Bi} (f) W_VMo_V, from DFT(GGA)+U calculations. The orange lines represent the total DOS (TDOS) black for O 2*p*, blue for V 3*d*, red for the quadruplicate of Mo 4*d* and magenta for the quadruplicate of W 5*d*, respectively. The Mo 4d and W 5d states are multiplied by 4 times to show their distribution clearly. The dashed lines stand for the Fermi level (at 0eV).

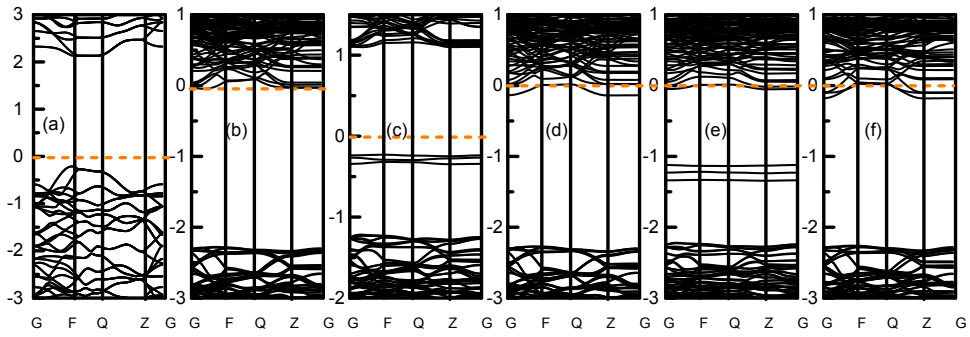

Fig. S4 Band structures of pure, Mo,W mono-doped and Mo/W co-doped $BiVO_4$: (a)pure, (b)W_V, (c)Mo_{Bi}, (d)Mo_V, (e) W_VMo_{Bi} (f) W_VMo_V, from DFT(GGA)+U calculations. The dashed lines stand for the Fermi level (at 0eV).

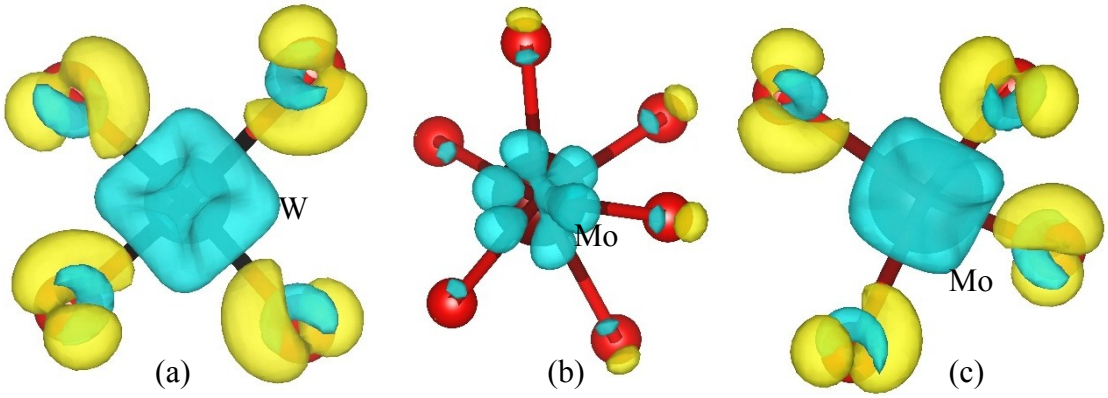

Fig S5 (Color online) Charge density difference isosurfaces of (a)W_V (b) Mo_{Bi} and (c)Mo_V mon-doped $BiVO_4$. The cyan region represents charge depletion and the yellow region represents charge accumulation. The isosurface value is 0.03 e/Å^3. The light red, purple and black spheres represent O, Mo and W atoms, respectively.