Supporting Information for:

Enhancing the photoelectrochemical activity of monoclinic $BiVO_4$ by discretizing oxygen vacancies: insights from DFT calculations

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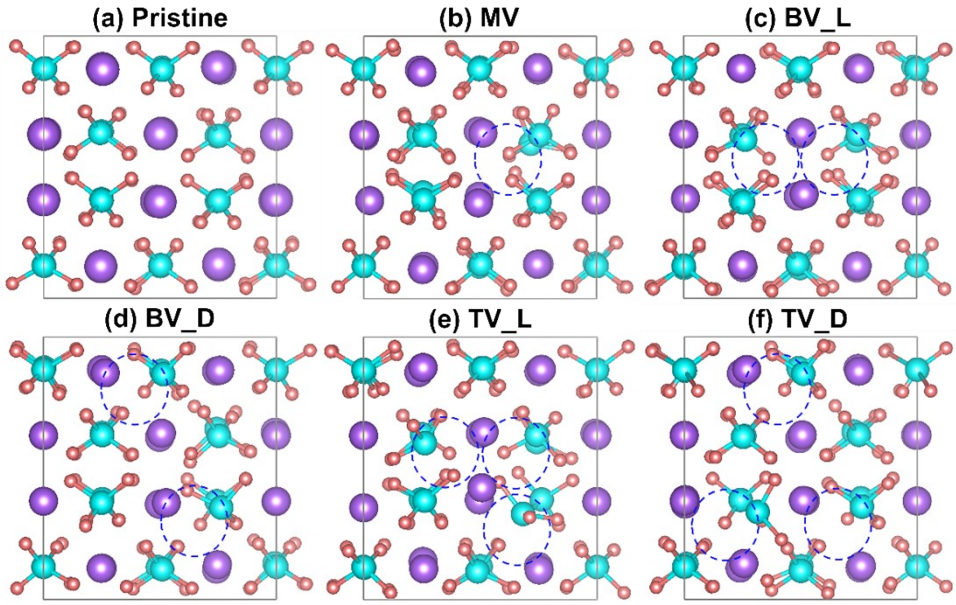

Fig. S1. Top view of the representative structures of the 3 ps MD trajectories.. (a) Pristine $BiVO_4$, (b) MV, (c) BV_L, (d) BV_D, (e) TV_L, (e) TV_D. The purple, cyan, and coral balls represent Bi, V, and O atoms, respectively. The oxygen vacancy positions are circled with a dotted line.

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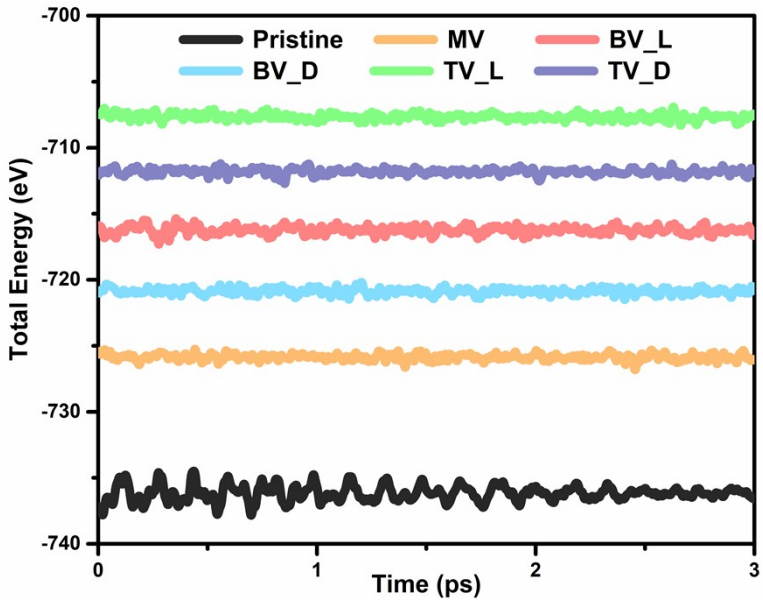

Fig. S2. Time-dependent total energies of the 3 ps MD trajectories for pristine $BiVO_4$, MV, BV_L, BV_D, TV_L, TV_D systems at room temperature.

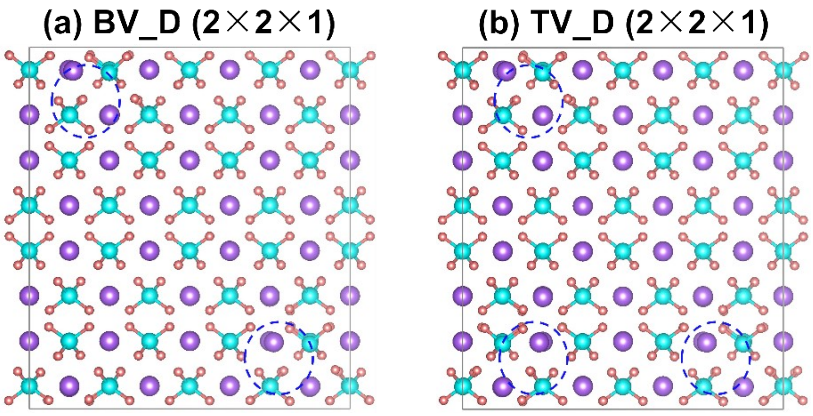

Fig. S3. Top view of the optimized geometries. (a) BV_D (2×2×1), (b) TV_D (2×2×1). The purple, cyan, and coral balls represent Bi, V, and O atoms, respectively. The oxygen vacancy positions are circled with a dotted line.

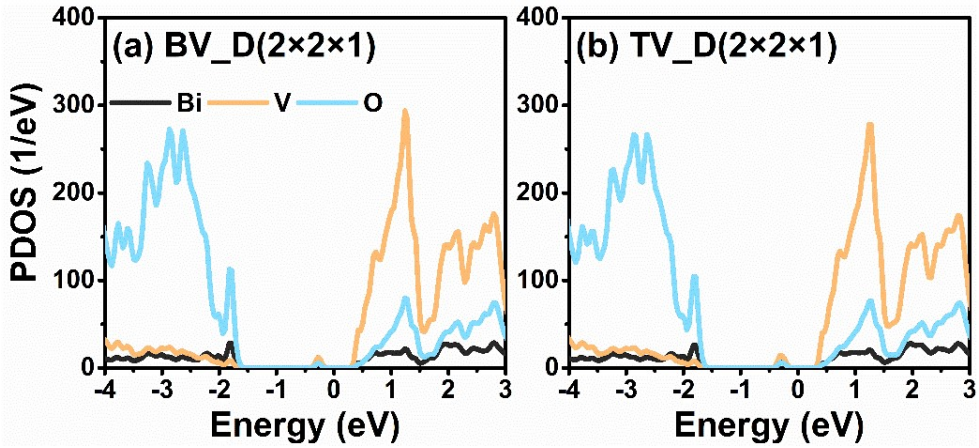

Fig. S4. Projected density of states (PDOS) calculated using the PBE function. (a) BV_D (2×2×1), (b) TV_D (2×2×1). The Fermi level is set to zero.

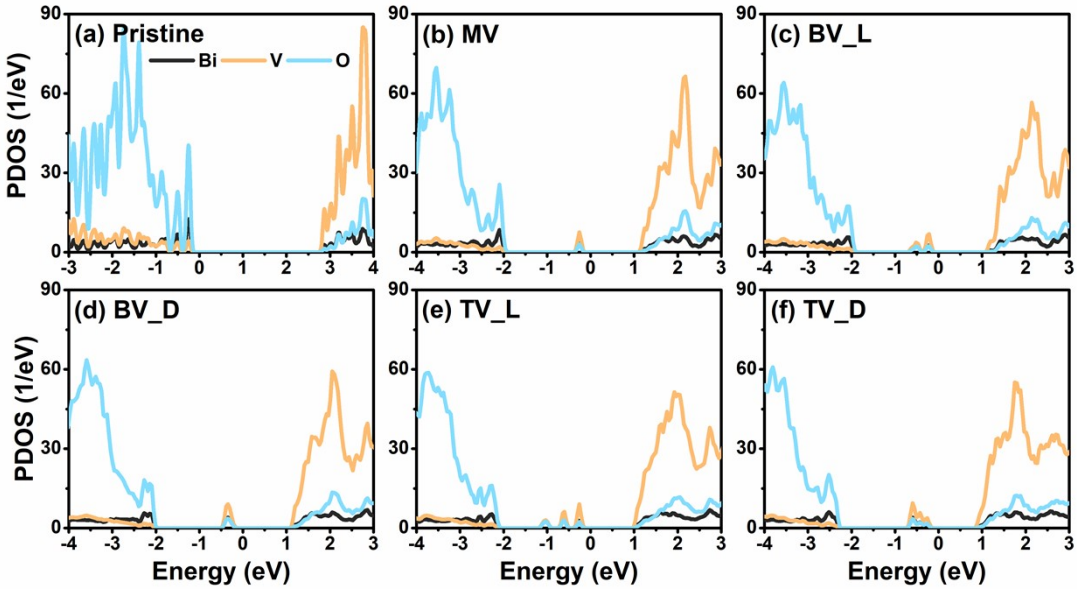

Fig. S5. Projected density of states (PDOS) calculated using the HSE06 function. (a) Pristine $BiVO_4$, (b) MV, (c) BV_L, (d) BV_D, (e) TV_L, (f) TV_D. The Fermi level is set to zero.