Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Charge transport, interfacial interactions and synergistic mechanism in $BiNbO_4/MWO_4$ (M = Zn and Cd) heterostructure for hydrogen production: insights from a DFT+*U* study

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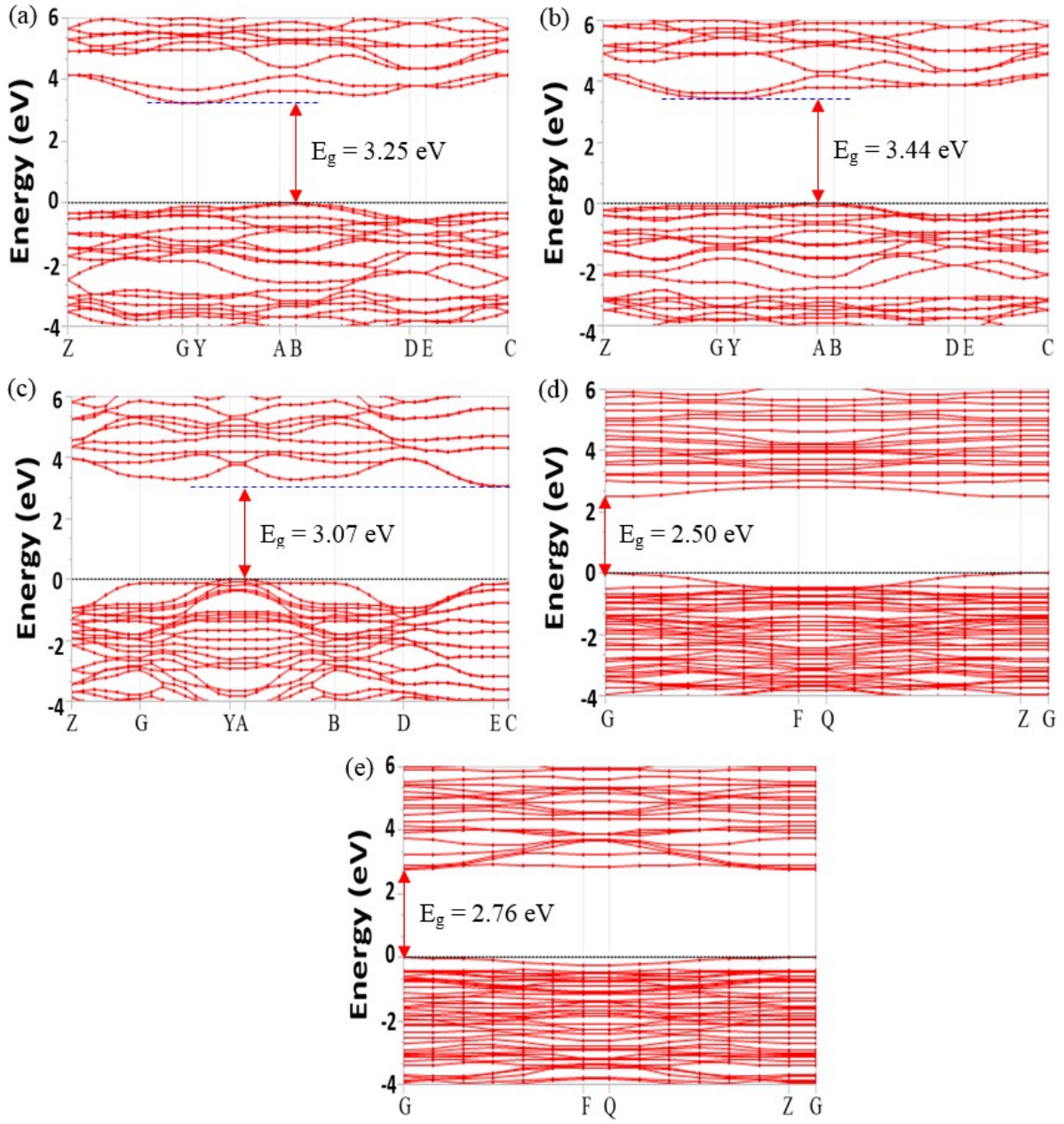

Fig. S1. Calculated unfolded band structure of (a) MoS_2(001), (b) WS_2(001), (c) MoS_2/*m*-$BiVO_4$(010) and (d) WS_2/*m*-$BiVO_4$(010) within the hybrid HSE06 functional. The Fermi level is set to zero as dashed horizontal black line.

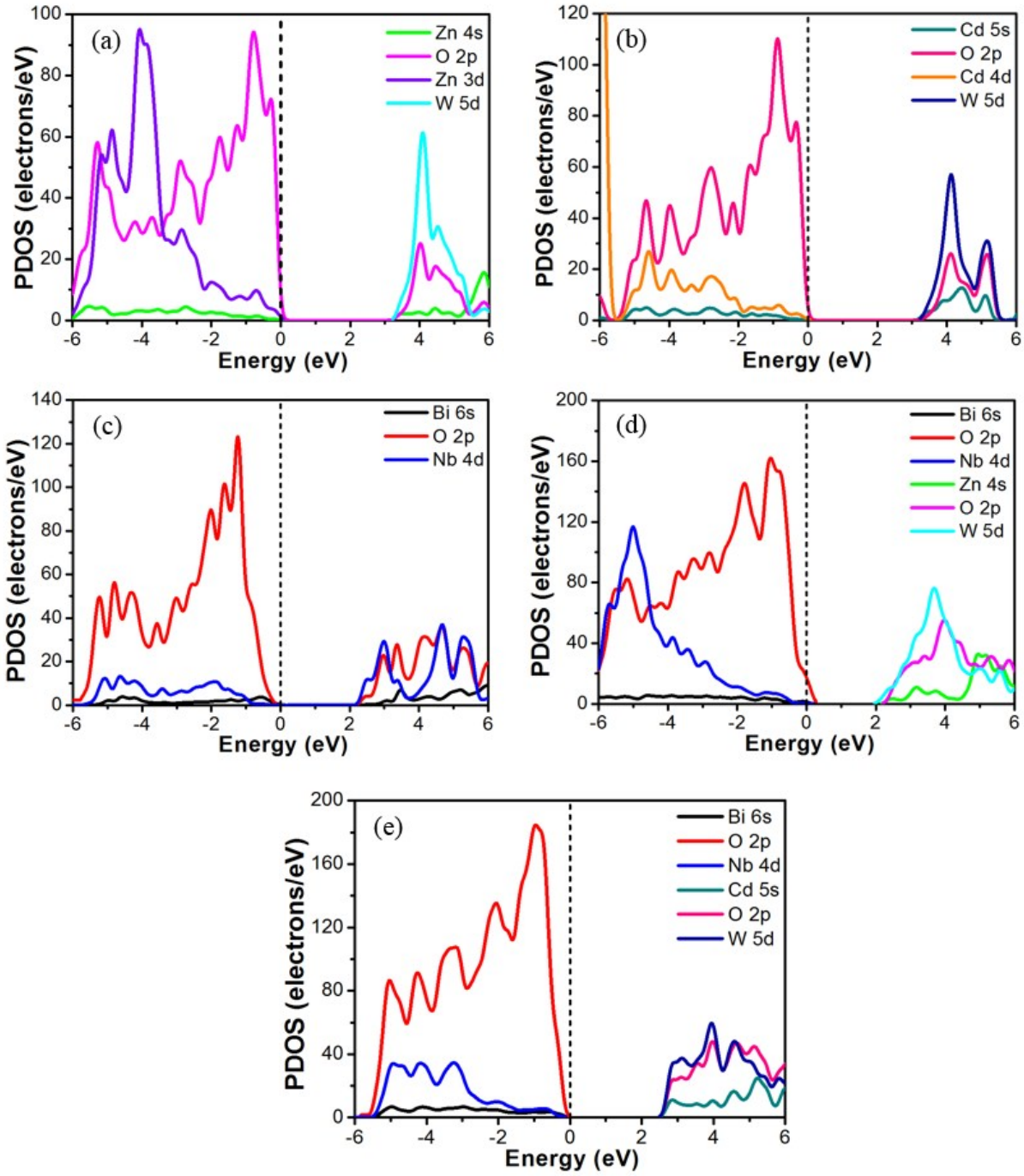

Fig. S2 GGA+*U* calculated PDOS of (a) $ZnWO_4$(010) surface, (b) $CdWO_4$(010) surface, (c) $BiNbO_4$(010) surface, (d) $BiNbO_4$/ $ZnWO_4$(010) heterostructure and (e) $BiNbO_4$/$CdWO_4$(010) heterostructure. The Fermi level is set to zero eV as a black dashed line.