Role of MoS$_2$ and WS$_2$ monolayers on the photocatalytic hydrogen production and pollutant degradation of monoclinic BiVO$_4$: a first-principles 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. Calculated PDOS 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 vertical dashed line is the Fermi level.
Fig. S3. The work function of the unfolded (a) MoS$_2$(001), (b) WS$_2$(001), (c) MoS$_2$/m-BiVO$_4$(010) and (d) WS$_2$/m-BiVO$_4$(010). The red and green dashed lines are the vacuum and Fermi level, respectively.