Stacking Tuning the Electronic and Optical Performances of the $MoTe_2/PtS_2$ Heterostructure as a Promising Photocatalyst in Water Splitting

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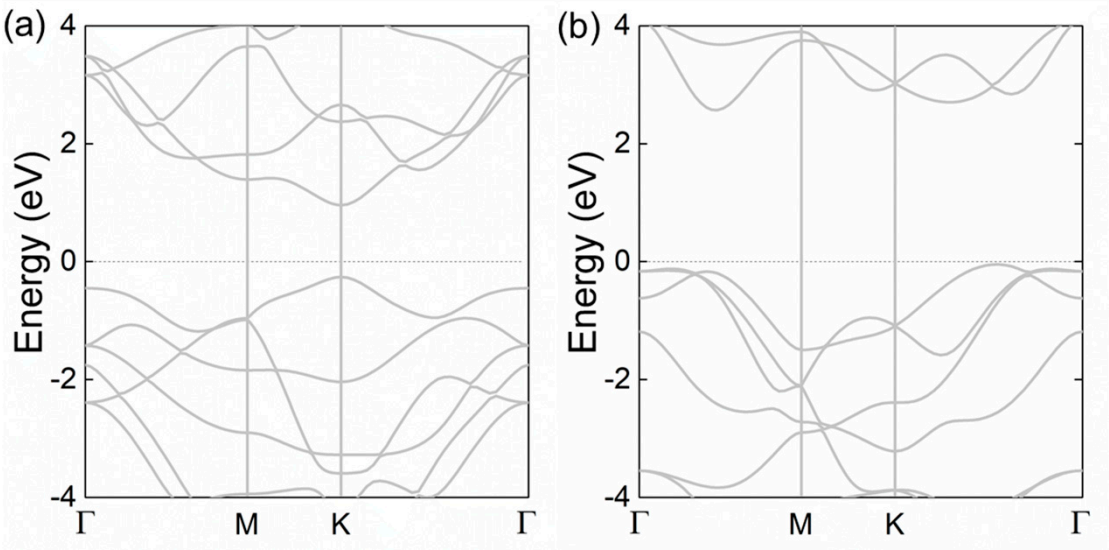

Figure. S1 The HSE06 calculated band structure of the (**a**) $MoTe_2$ and (**b**) PtS_2 monolayers. The Fermi level is set as 0 eV.

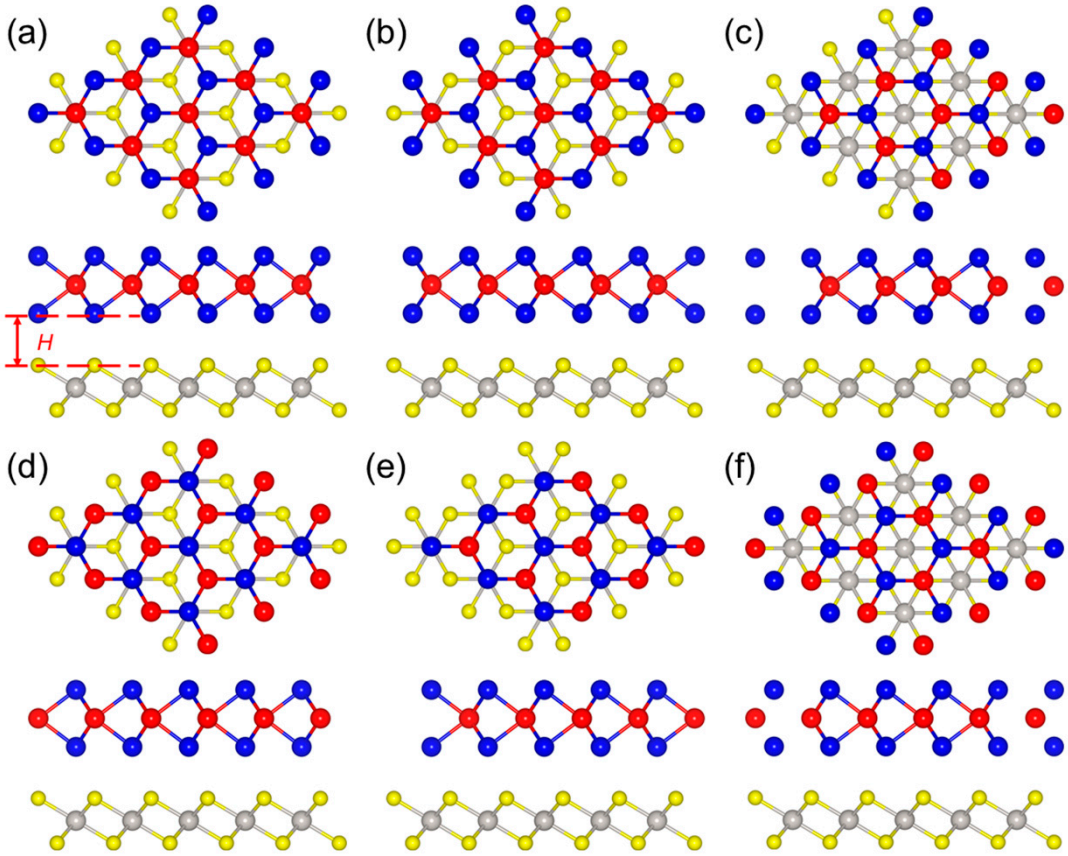

Figure. S2 The $MoTe_2/PtS_2$ heterostructure constructed by (**a**) P1, (**b**) P2, (**c**) P3, (**d**) P4, (**e**) P5 and (**f**) P6 stacking configurations. The yellow, gray, red, and blue balls represent S, Pt, Mo, and Te atoms, respectively.