Supporting Information for

Designed Borophene/TMDs Hybrid Catalysts for Enhanced Hydrogen Evolution Reaction

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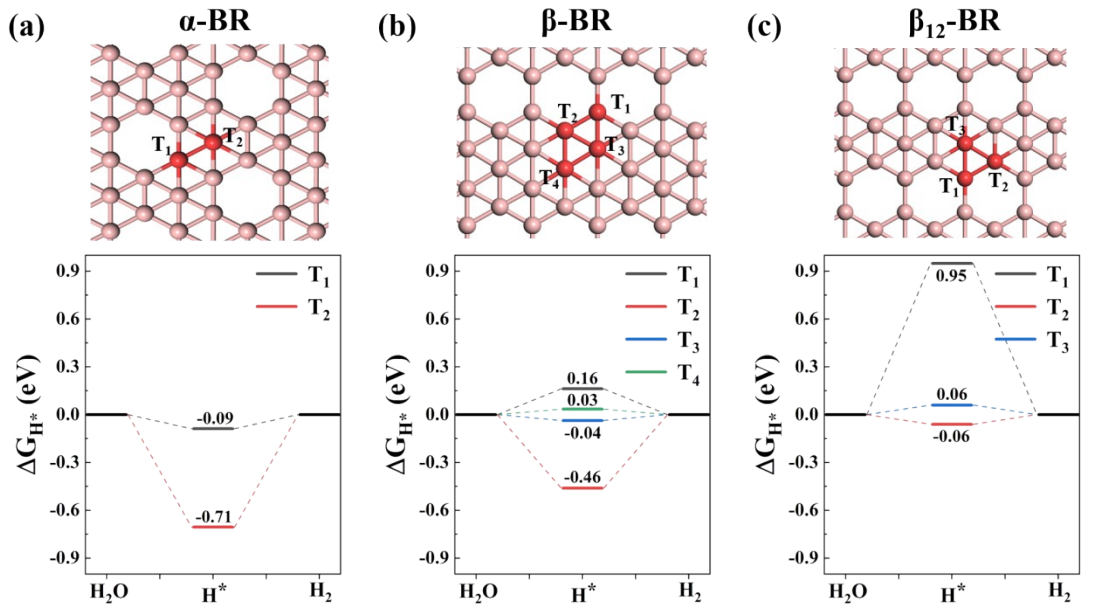

Figure S1. Adsorption free energies of H atoms on freestanding (a) α-BR, (b) β-BR and (c) β_{12}-BR. Insets are the structure of α-BR, β-BR, and β_{12}-BR sheet, T_1, T_2, T_3, T_4 refers to the H adsorption site.

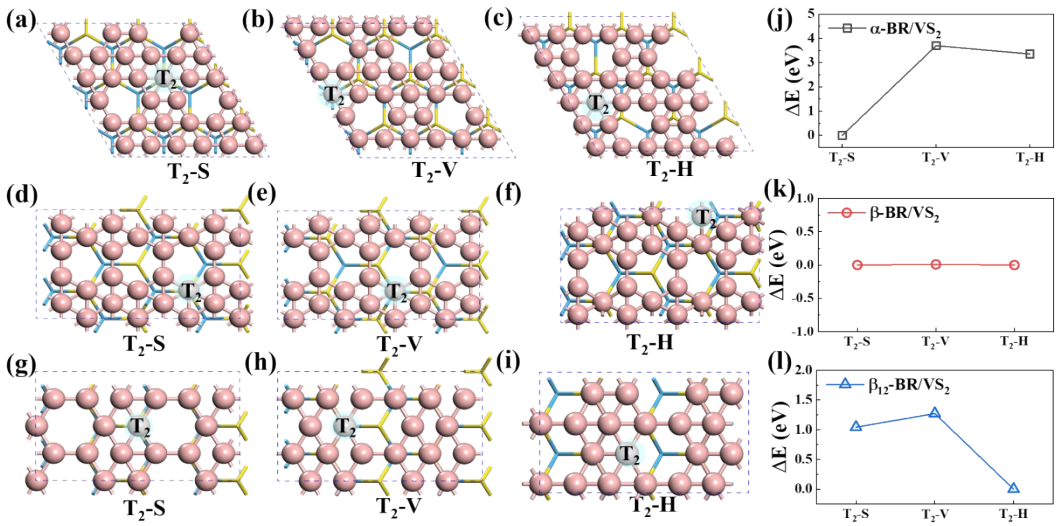

Figure S2. The structures (a-i) and relative energies(j-l) of α-BR/VS_2, β-BR/VS_2 and β_{12}-BR/VS_2 with three types of interlayer stackings: (a, d, g) T_2-S, (b, e, h) T_2-V and (g, h, i) T_2-H.

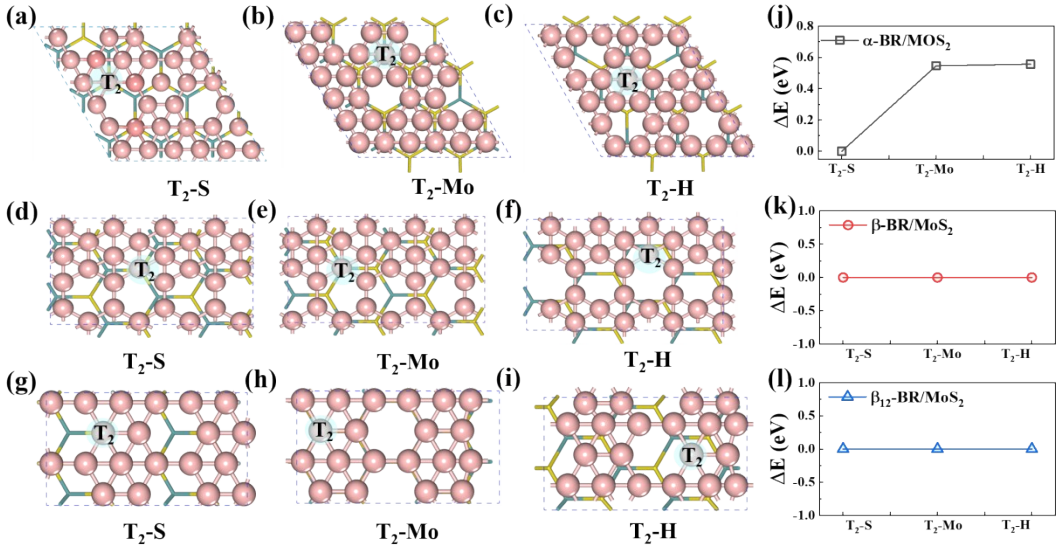

Figure S3. The structures (a-i) and relative energies(j-l) of α-BR/MoS_2, β-BR/MoS_2 and β_{12}-BR/MoS_2 with three types of interlayer stackings: (a, d, g) T_2-S, (b, e, h) T_2-V and (g, h, i) T_2-H.

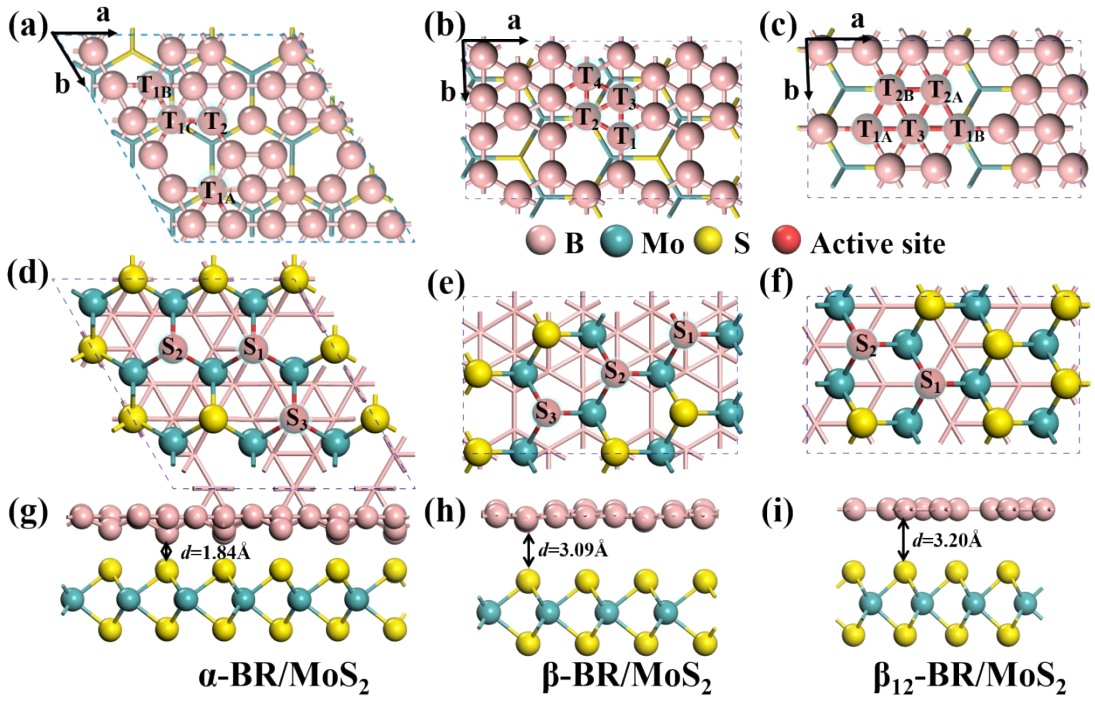

Figure S4. Top (up-side/down-side) and side views of α-BR/MoS_2 (a, d, g), β-BR/MoS_2 (b, e, h) and β_{12}-BR/MoS_2 (c, f, i) heterostructures.

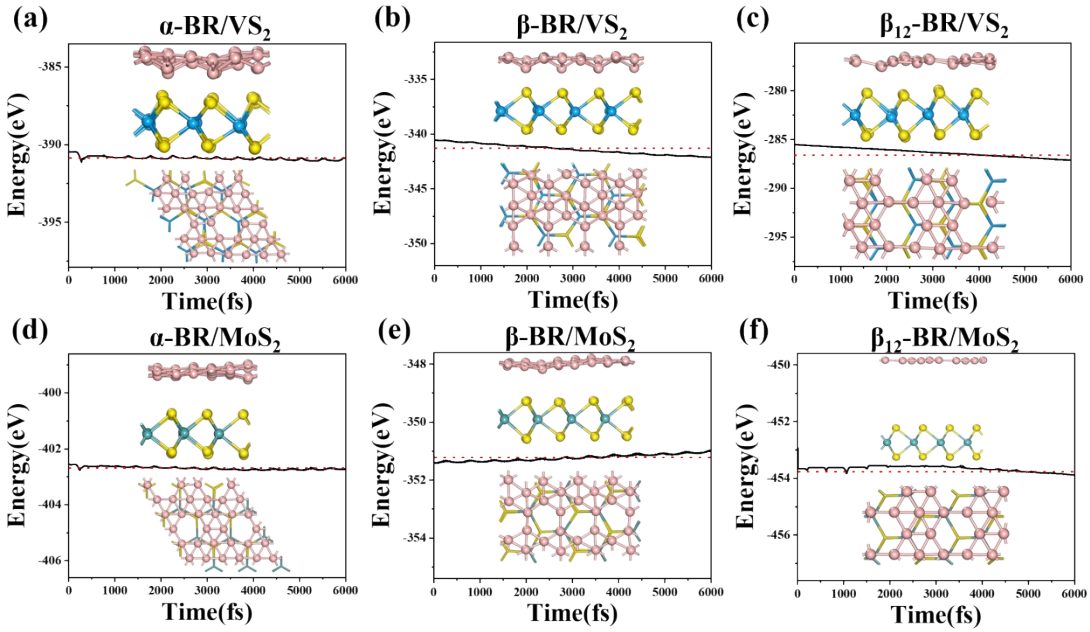

Figure S5. Variations of energies and geometries against the time for AIMD simulations. The simulation is run at 300K for 6000fs.

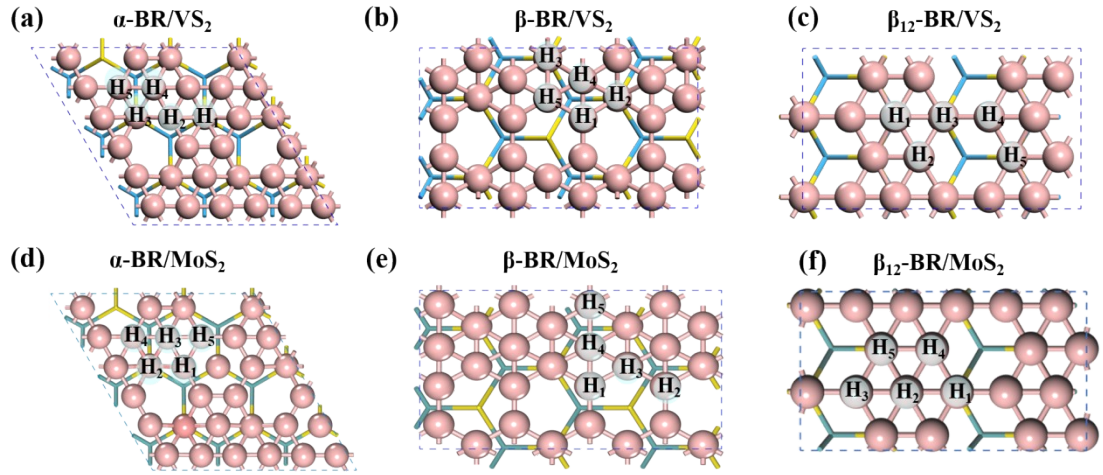

Figure S6. (a-f) Scheme of 1H-5H adsorption on the Borophene sublayer.

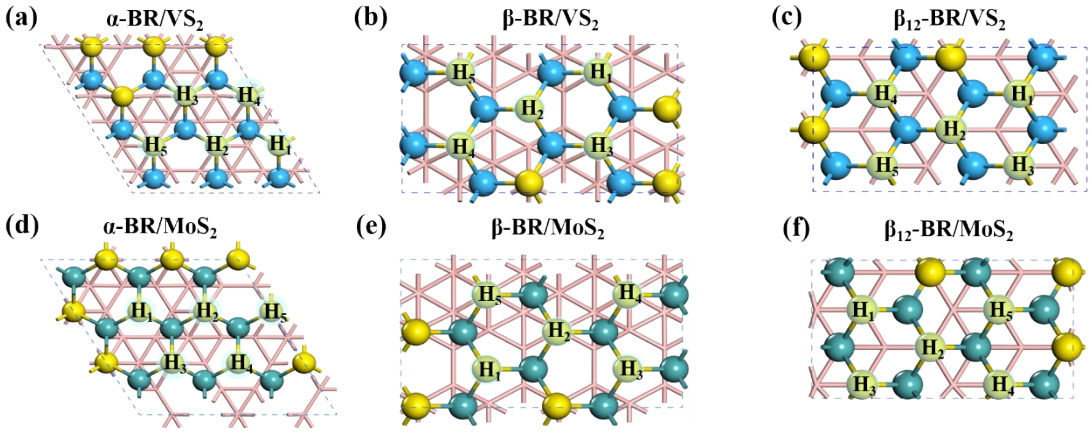

Figure S7. (a-f) Scheme of 1H-5H adsorption on the TMS_2 sublayer.

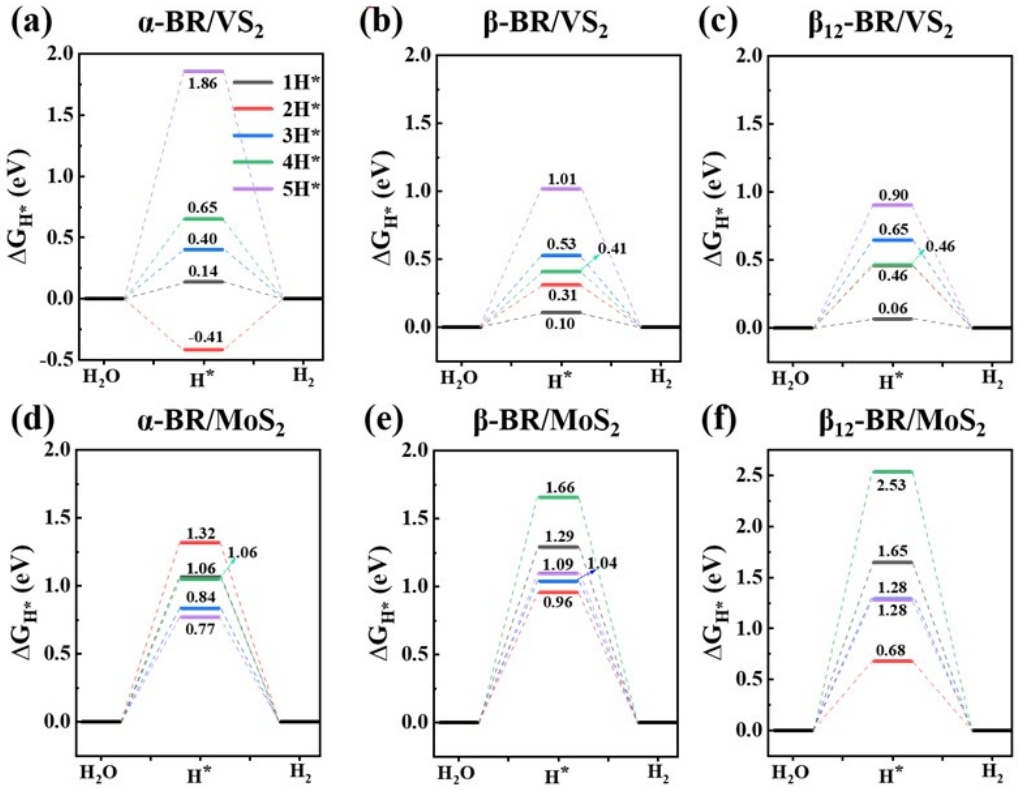

Figure S8. The free energies of H atoms on S sites of BR/TMDs at different H coverage.

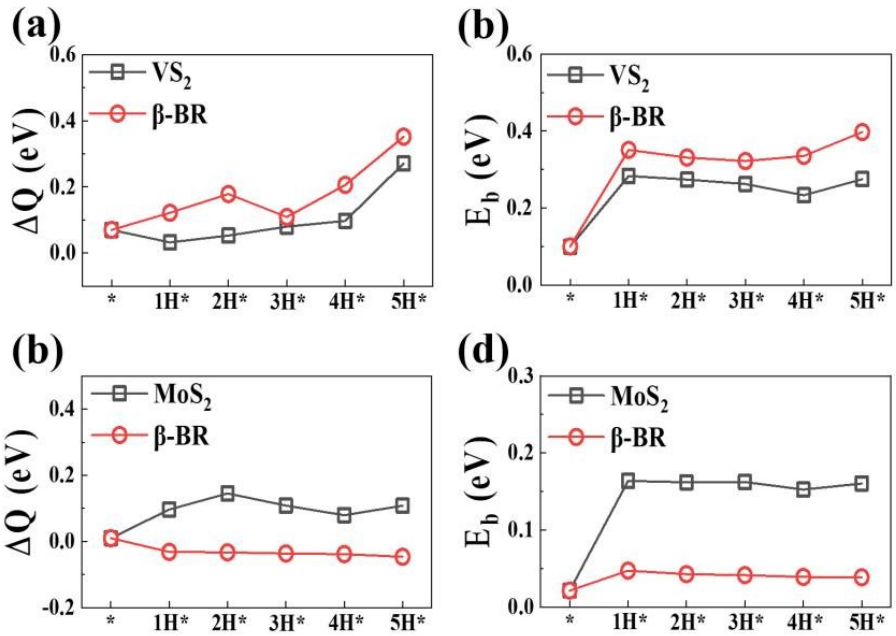

Figure S9. The interlayer binding energies and charges transfer of β-BR/TMS_2 (TM=V, Mo) with different H coverage.

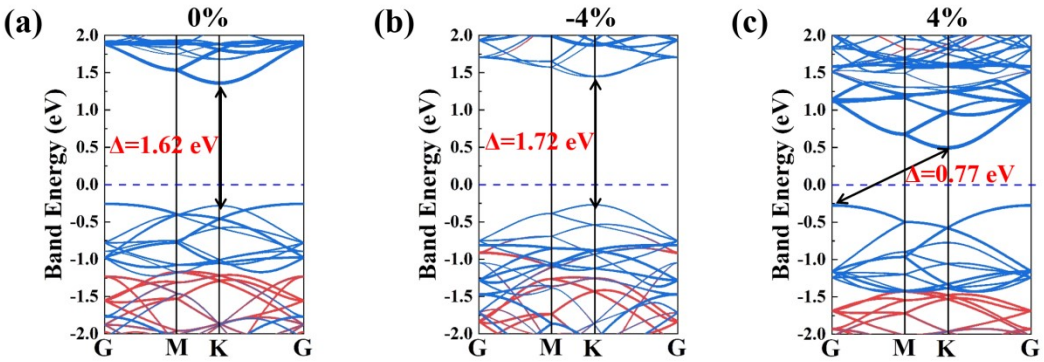

Figure S10. Electronic band structures of MoS_2 monolayer under (a) 0%, (b) -4% and (a) 4% strain. The red and blue lines denote the electronic states of S atom and Mo atom of MoS_2 monolayer,, respectively.