

Figure S1 (a) Side view of the LUMO and HOMO of the GaTe/PtS<sub>2</sub> heterojunction, with the isosurface value of 0.005e Å<sup>-3</sup>.

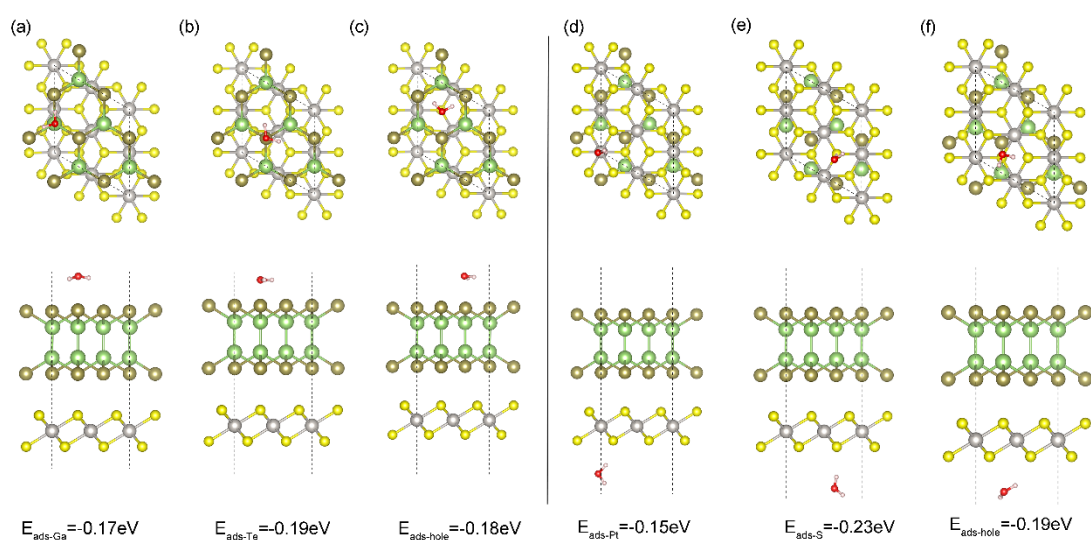


Figure S2 The relaxed structures and adsorption energies of adsorbed H<sub>2</sub>O molecules at different sites on (a)-(c) GaTe surface and (d)-(f) PtS<sub>2</sub> surface, respectively.