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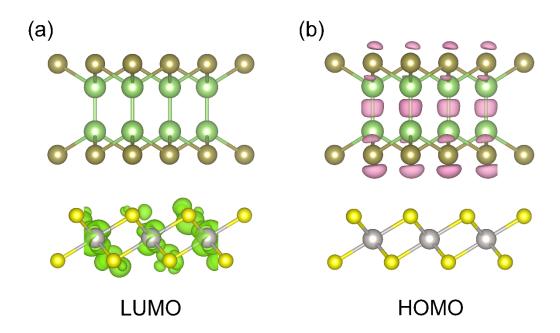


Figure S1 (a) Side view of the LUMO and HOMO of the GaTe/PtS2 heterojunction, with the isosurface value of $0.005e~{\rm \AA}^{-3}$.

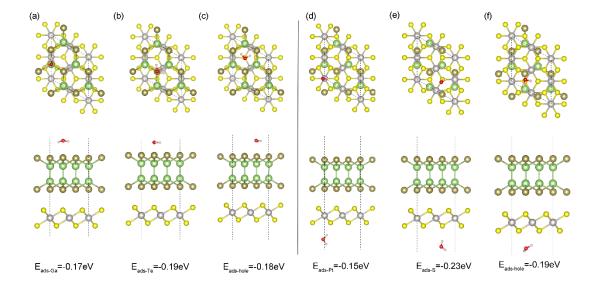


Figure S2 The relaxed structures and adsorption energies of adsorbed H₂O molecules at different sites on (a)-(c) GaTe surface and (d)-(f) PtS₂ surface, respectively.