Supplementary Information:

Strain Effects on Phase Transitions in Transition Metal Dichalcogenides

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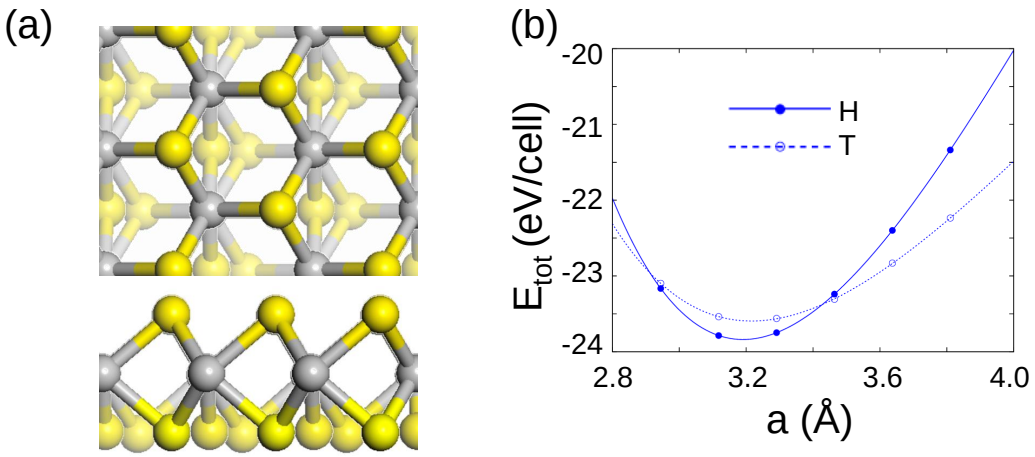

Figure S1: (a) Illustration of three steps of a considered phase transition pathway from the *T* phase to the *H* phase: top and side views. (b) Total Energy E_{tot} of the *H* (solid line) and *T* (dotted line) phases of WS_2 as a function of lattice constants calculated with spin-orbit coupling.

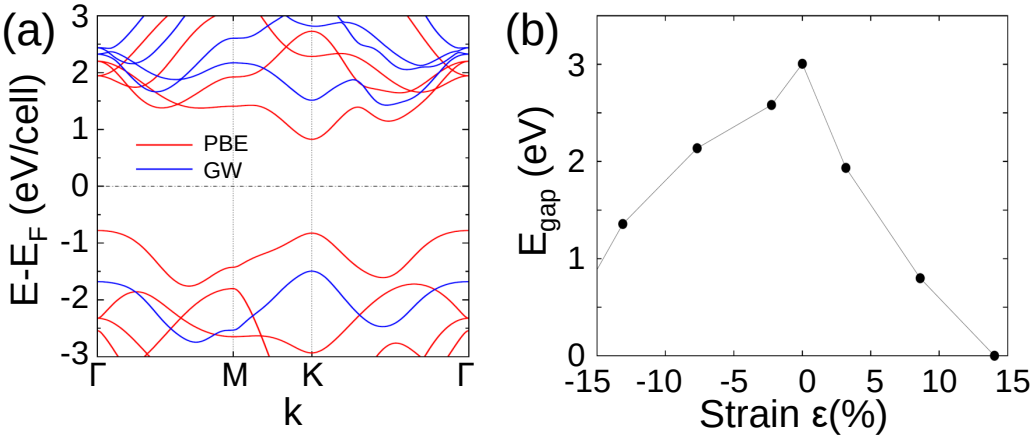

Figure S2: (a) Electronic band structures of the *H*-phase MoS_2 at equilibrium obtained from PBE functional (red) and *GW* correction (blue). (b) Electronic band gap as function of strain in the *H*-phase MoS_2 within *GW* correction.