Supporting Information for "Strain engineering of two-dimensional piezo-photocatalytic materials for improved hydrogen evolution reaction"

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Keywords: piezo-photocatalysis, transition metal dichalcogenides, strain engineering, hydrogen production, density functional theory

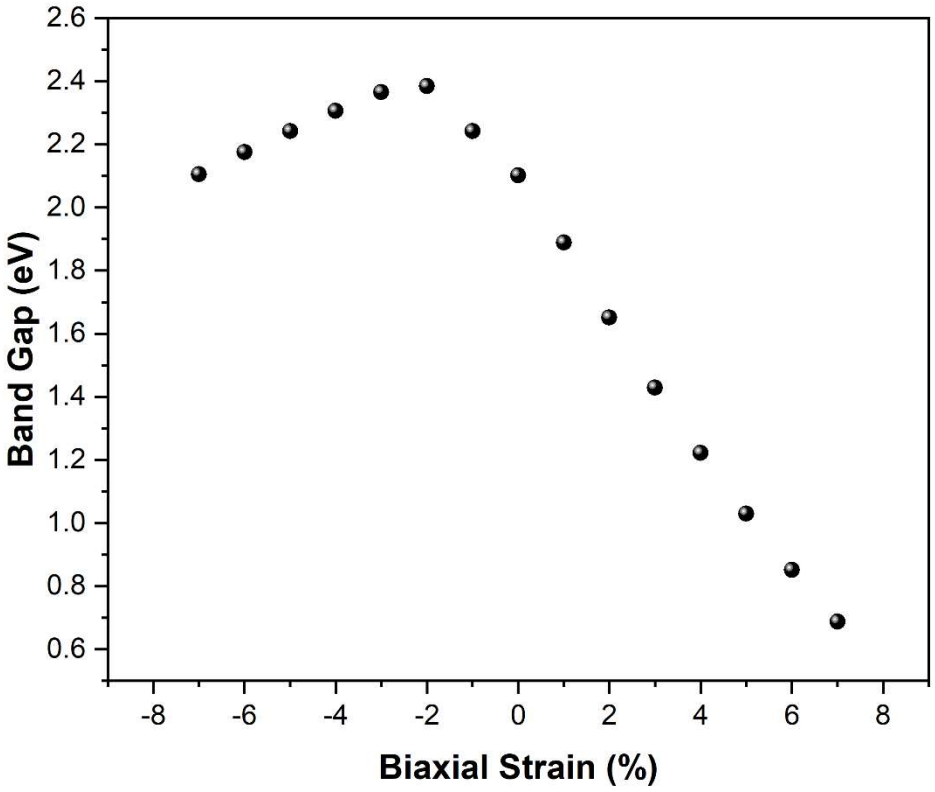

Figure S1. Strain-induced band gap evolution of the 2H MoS_2 monolayer expressed as a function of epitaxial strain. The results were obtained with the hybrid HSE06 DFT functional.

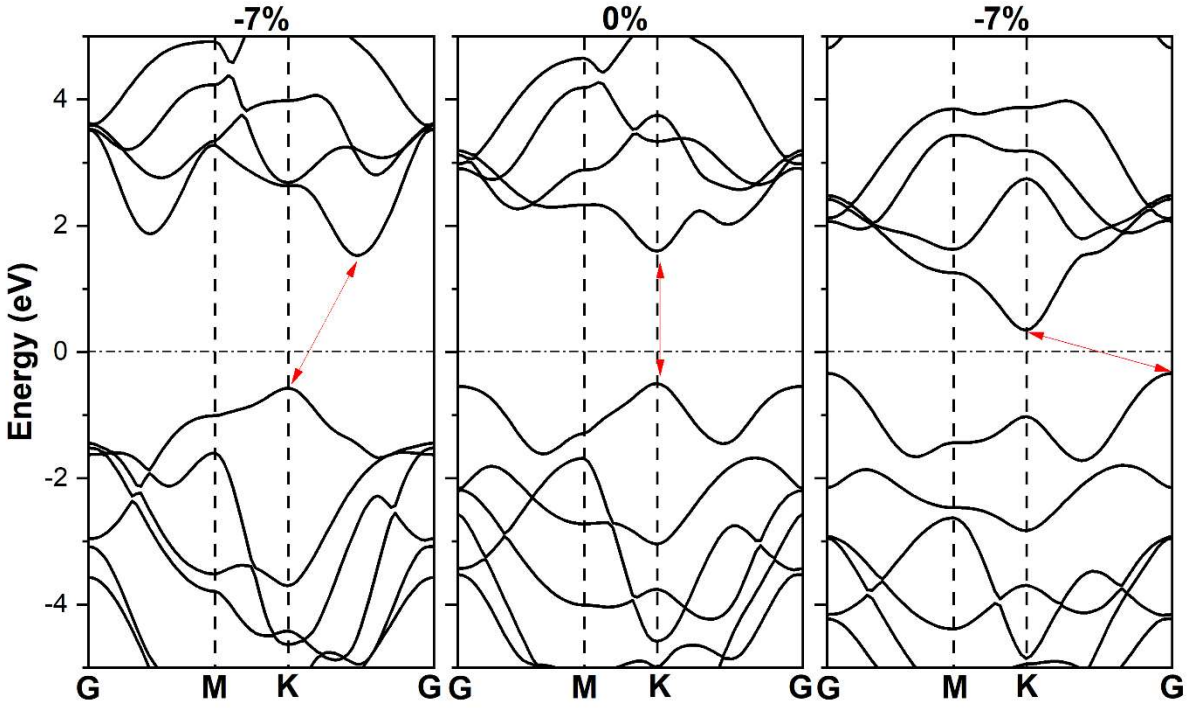

Figure S2. Calculated band structure of the 2H MoS_2 monolayer calculated as a function of epitaxial strain. The results were obtained with the hybrid HSE06 DFT functional.

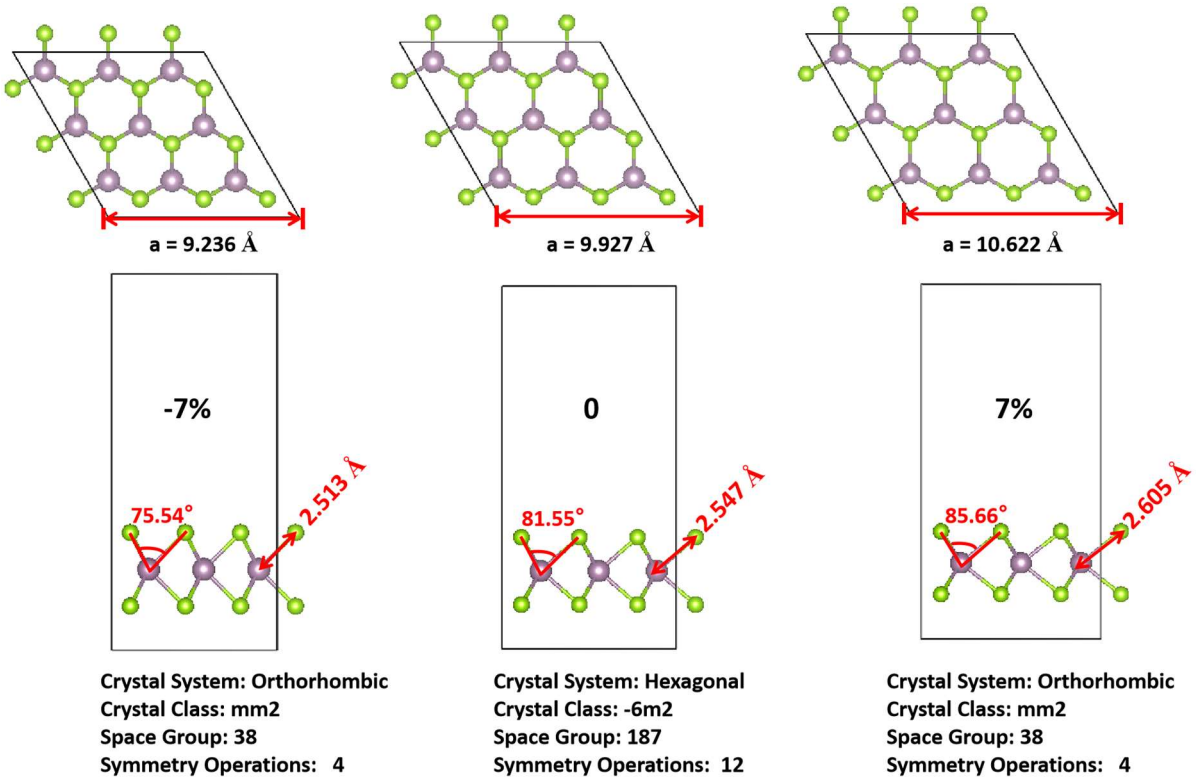

Figure S3. Crystalline symmetry changes in 2H TMDC monolayers as induced by epitaxial strain.

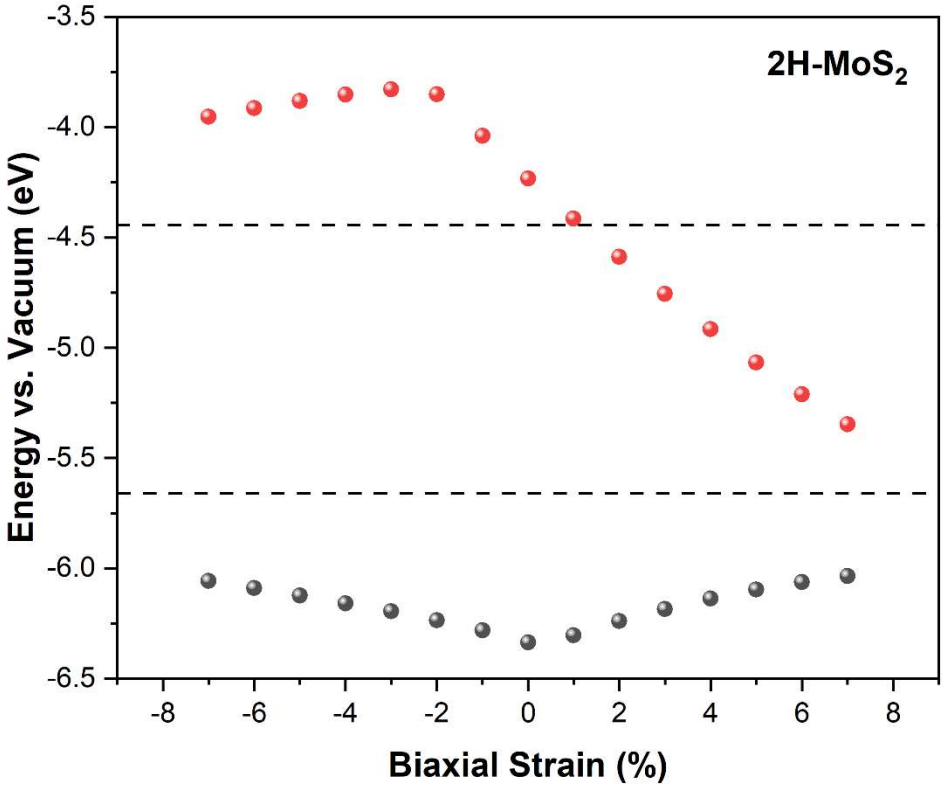

Figure S4. Calculated band alignments of the 2H MoS_2 monolayer estimated as a function of epitaxial strain. Red and black dots represent the CBM and VBM levels, respectively. The results were obtained with the hybrid HSE06 DFT functional.

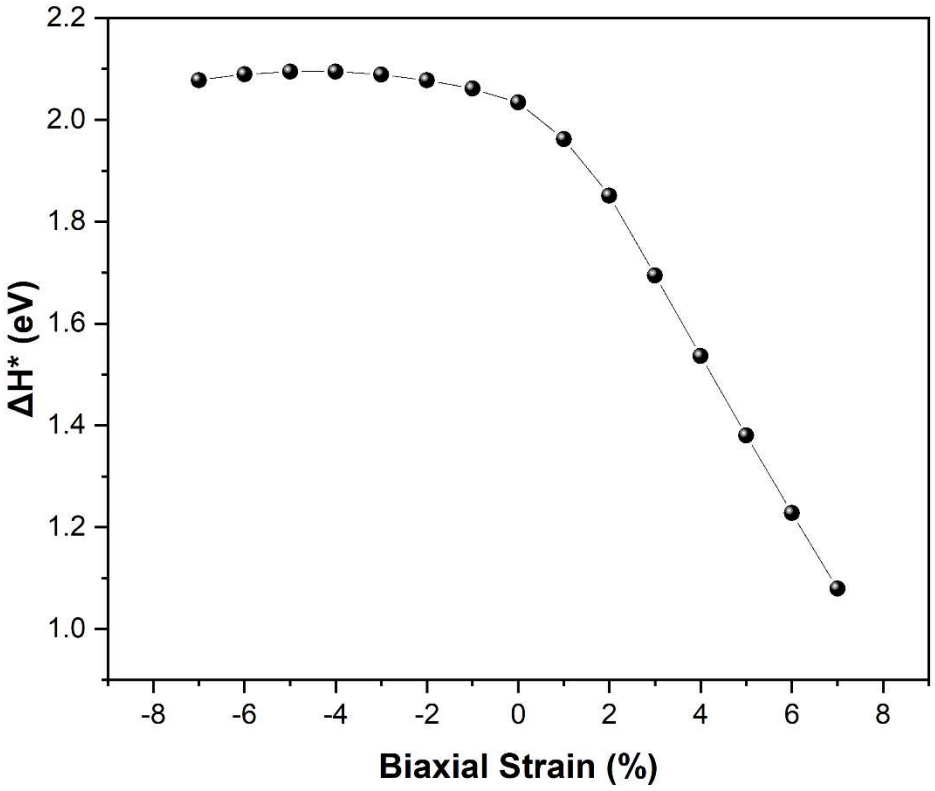

Figure S5. Calculated H adsorption free energies expressed as a function of epitaxial strain for the 2H MoS_2 monolayer. The results were obtained with the semi-local PBE DFT functional.

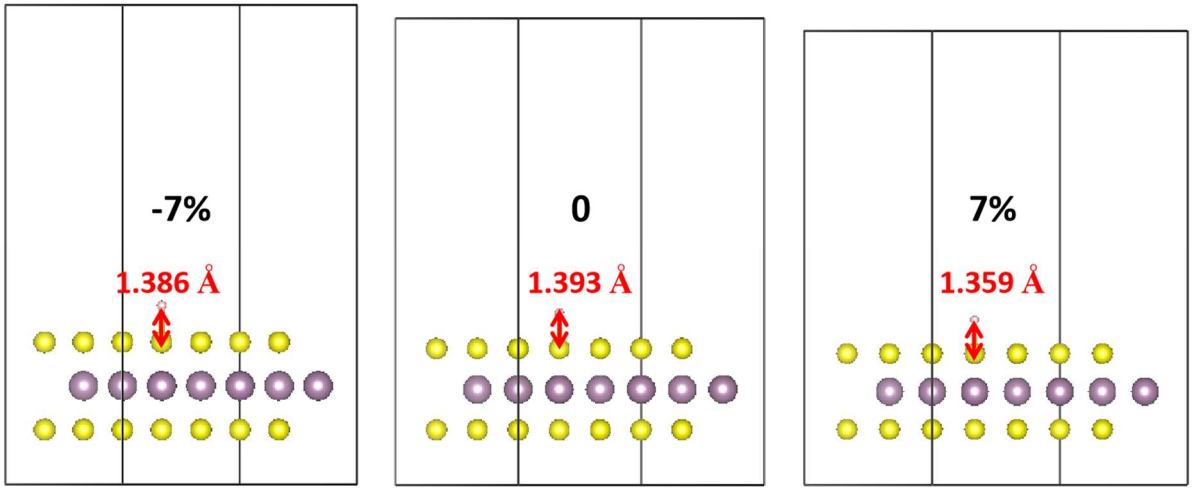

Figure S6. Adsorption of an H atom on the 2H MoS_2 monolayer under different biaxial strain conditions.

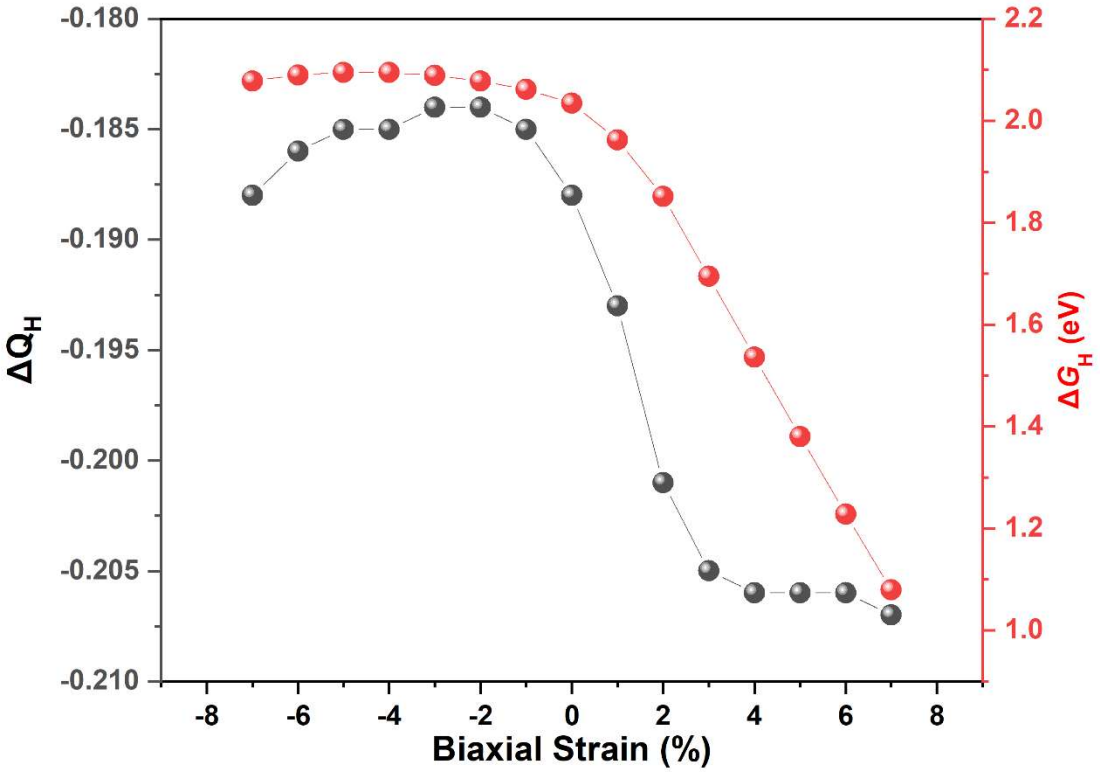

Figure S7. Comparison of the ΔQ_H (electronic charge difference between the H atom on the TMDC surface and the free H atom) and ΔG_H (H adsorption free energy) quantities obtained for the 2H MoS_2 monolayer and expressed as a function of epitaxial strain.