

Supporting Information
**Strain-Tunable ZrS₂-1H/ZrS₂-1T van der Waals Heterostructures with Quasi Type-II
Band Alignment for Solar Oxygen Evolution and Optoelectronic Applications**

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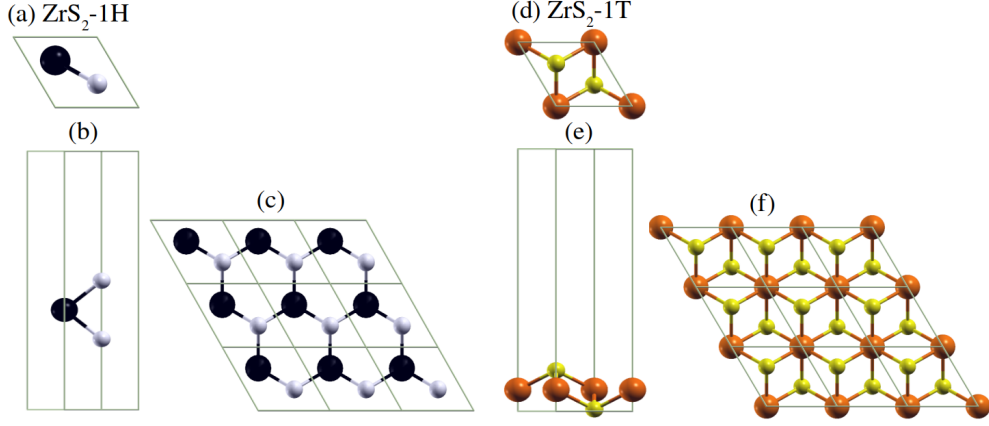


Figure 1: Ball and Stick model for different phases of ZrS_2 monolayers from side and top perspectives. (a-c) ZrS_2 -1H phase (d-f) ZrS_2 -1T phase. The black and white sphere represent Zr and S atoms in 1H monolayer, while orange and yellow spheres represents Zr and S atoms in 1T monolayers, respectively.

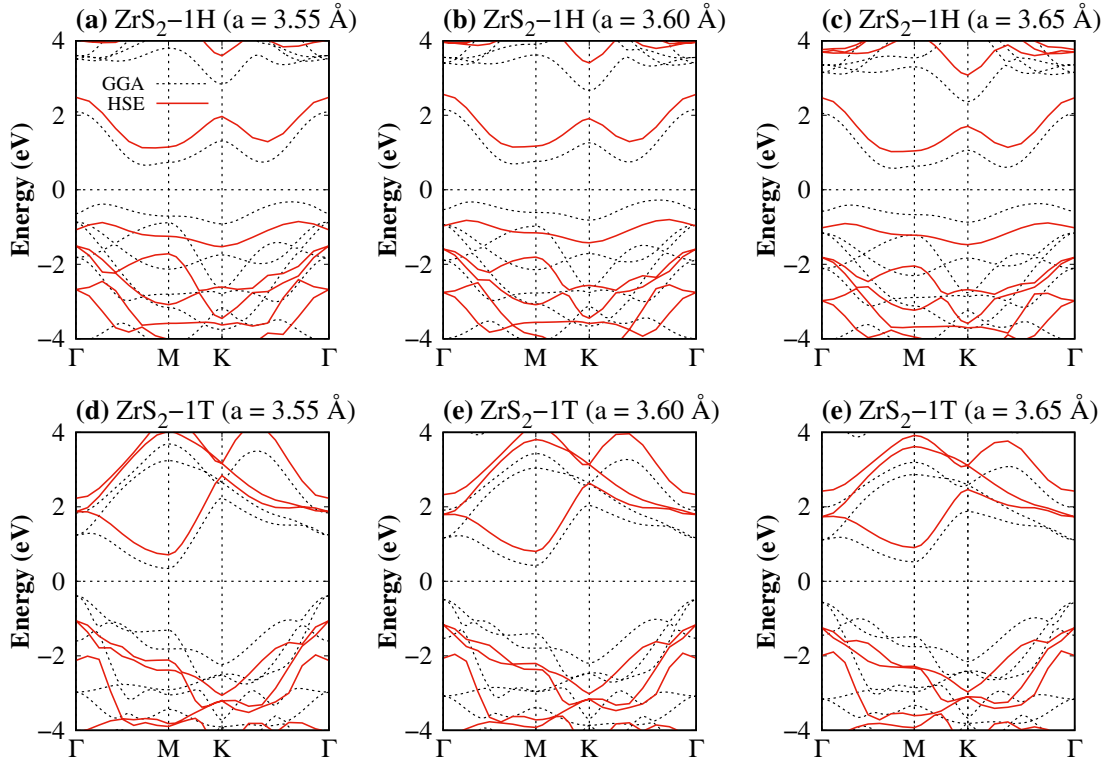


Figure 2: GGA and HSE06 calculated electronic band structures of ZrS_2 -1H and ZrS_2 -1T monolayers are illustrated for different equilibrium and biaxial strain (a) ZrS_2 -1H ($a = 3.55 \text{ \AA}$), (b) ZrS_2 -1H ($a = 3.60 \text{ \AA}$), (c) ZrS_2 -1H ($a = 3.65 \text{ \AA}$) (d) ZrS_2 -1T ($a = 3.55 \text{ \AA}$) (e) ZrS_2 -1T ($a = 3.60 \text{ \AA}$) (f) ZrS_2 -1T ($a = 3.65 \text{ \AA}$). The black dotted and red solid line indicates the band structure calculated using GGA and HSE06 energy functional. The Fermi level is set at zero axis.