Online supporting information for:

Mechanism of Hydrogen Evolution Reaction on 1T-MoS_2 from First Principles

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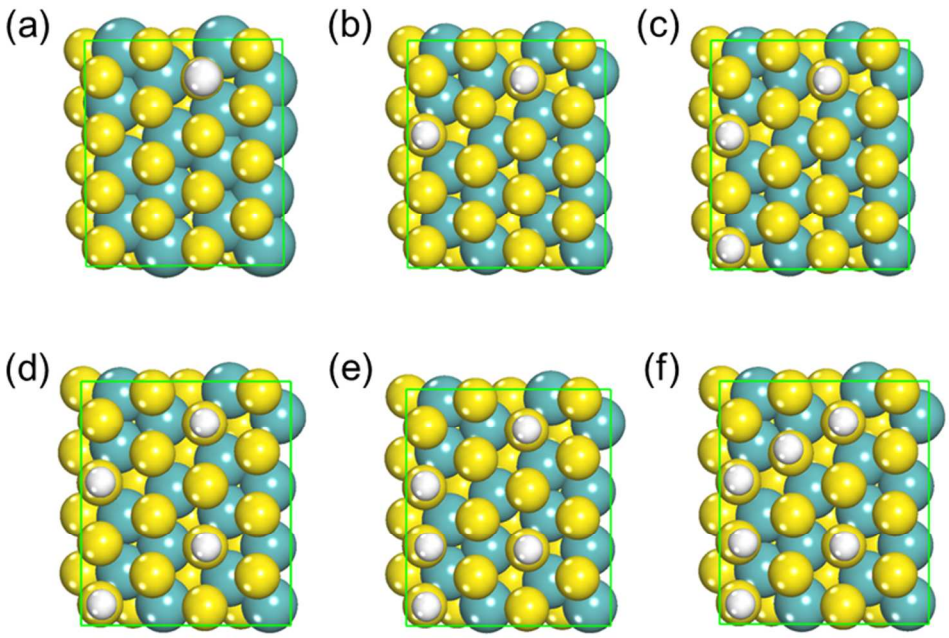

Figure S1. The optimized adsorption geometries of H on 1T MoS_2 surface at different H coverage: (a) 6.25 %, (b) 12.5%, (c) 18.75%, (d) 25%, (e) 31.25% and (f) 37.5%.

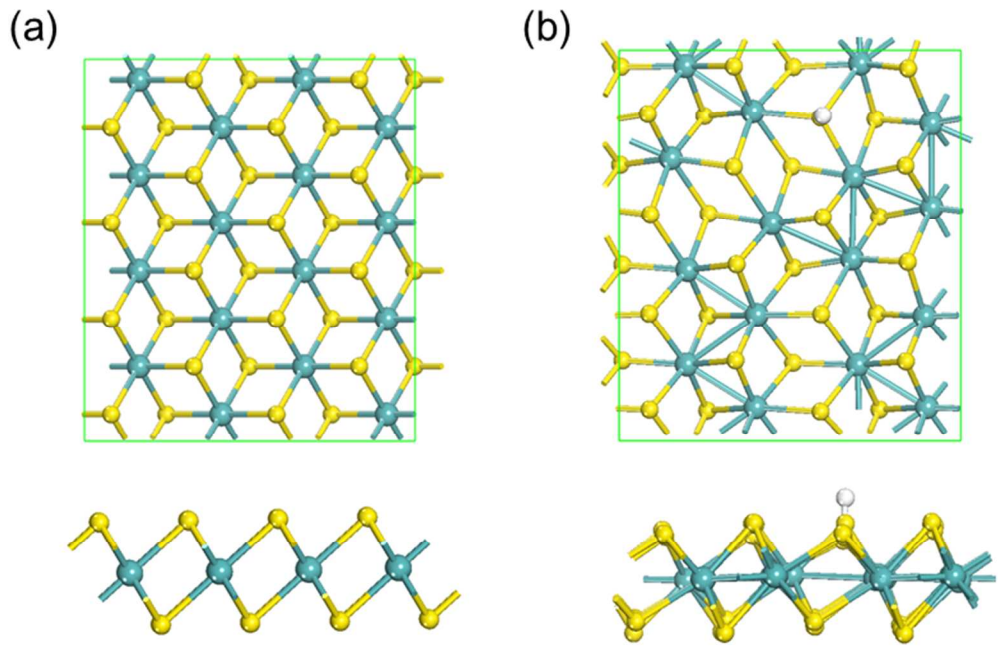

Figure S2. Top and side view of the perfect 1T MoS_2 (a) and the distorted 1T MoS_2 after adsorption of the first H.