Electronic Supplementary Material (ESI) for Catalysis Science & Technology.

Supplemental info to "A Comparative Study of Hydrogen Evolution Reaction on WS_2 and PtS_2 pseudo-monolayer: Insight based on Density Functional Theory"

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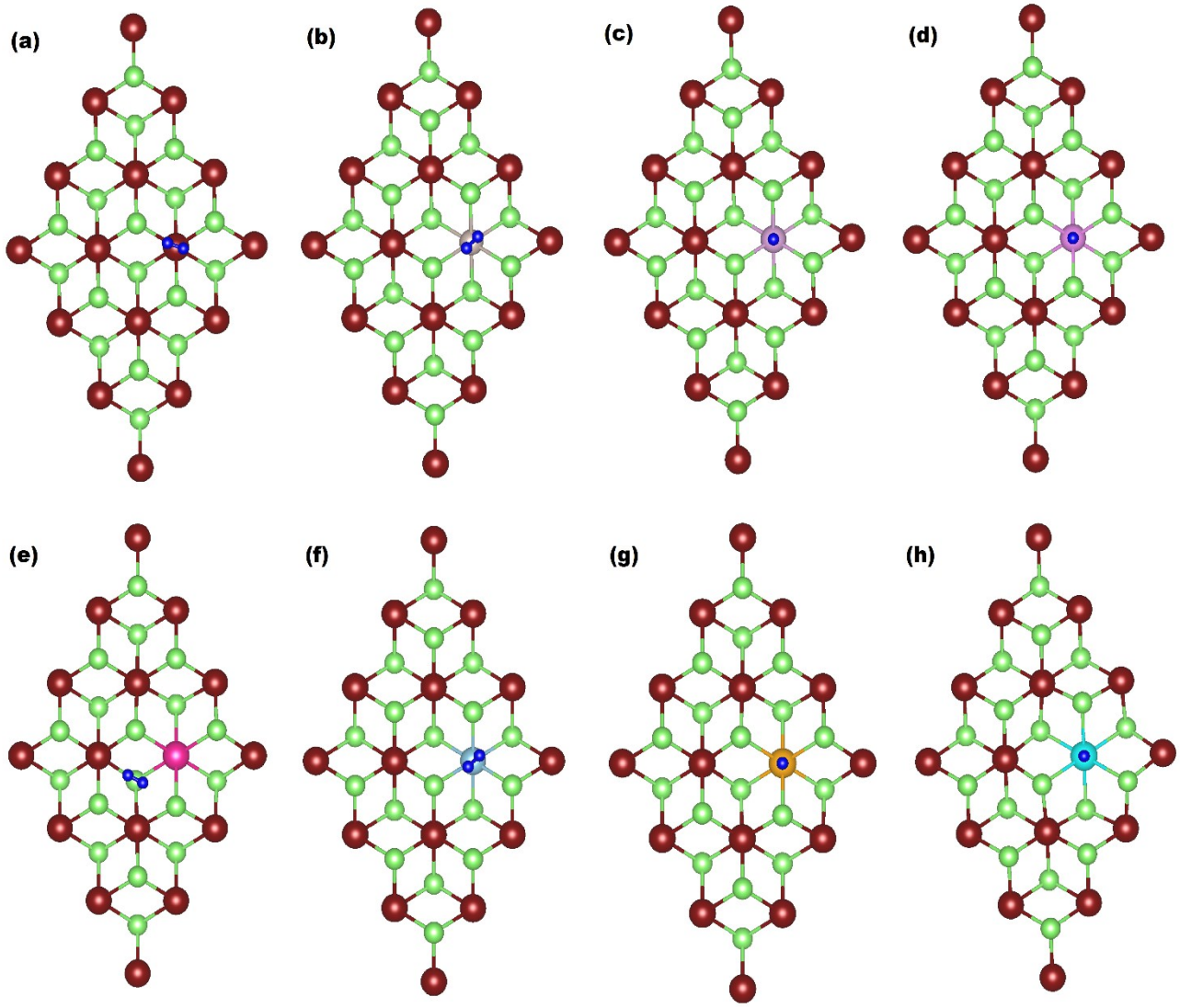

Fig. S1. The optimised geometries of H_2 on pristine (a) and functionalised PtS_2. (b), (c), (d), (e), (f), (g), and (h) represents systems doped with Ru, Rh, Pd, Ag, Ir, Au and Hg respectively. The optimised geometries shown have been calculated with VDW interactions taken into account. The colour of the elements is designated as follows: maroon for Pt, Red for W, green for S, grey for Ru, plum for Rh, violet for Pd, deep pink for Ag, sky blue for Ir, orange for Au and cyan for Hg.

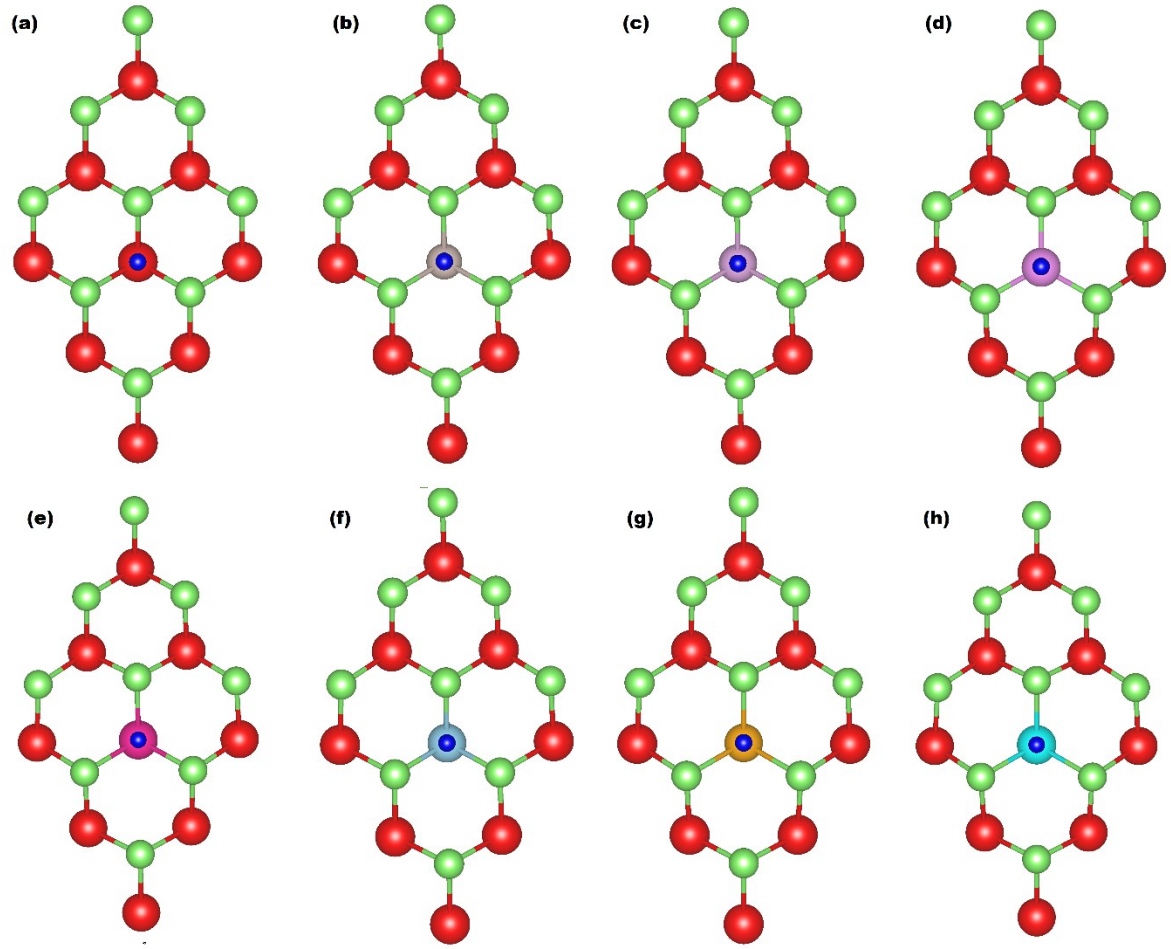

Fig. S2. The optimised geometries of H_2 on pristine (a) and functionalised WS_2. (b), (c), (d), (e), (f), (g), and (h) represents systems doped with Ru, Rh, Pd, Ag, Ir, Au and Hg respectively. The optimised geometries shown have been calculated with VDW interactions taken into account. The colour of the elements is designated as follows: maroon for Pt, Red for W, green for S, grey for Ru, plum for Rh, violet for Pd, deep pink for Ag, sky blue for Ir, orange for Au and cyan for Hg.