Supplementary Information for

Identification of electronic descriptor for catalytic activity of transition-metal and non-metal doped MoS_2

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PBE functional tends to underestimate the band gap compared to HSE. However, we have carefully checked TM doped MoS_2 calculated by both functionals and found that the band shape is not changed, and the resulting p-band center has only a collective shift as examples shown below (Fig. S1), which does not affect our results. In Fig. S2, we have shown the HSE06 calculated PDOS for comparison with Fig. 2a in our manuscript, where the band shape and the pining of the Fermi level upon doping are consistent with PBE calculated PDOS.

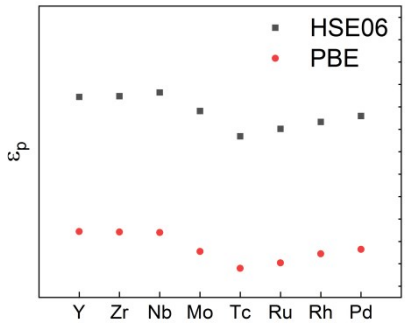

Figure S1. The collective shift of the p-band center calculated by HSE06 compared with PBE functional.

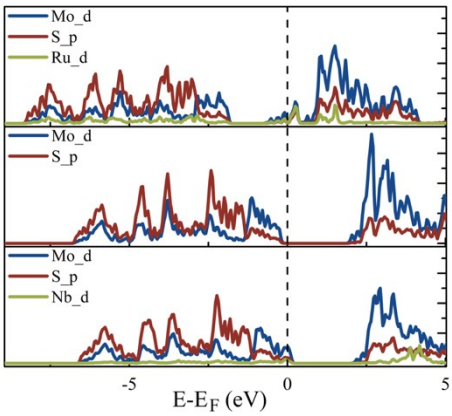

Fig. S2. PDOS of Ru doped, undoped, and Nb doped MoS_2 showing the change of DOS at band edges and the shift of the Fermi level calculated by HSE06.