## First Principles Study on 2H-1T' Transition in MoS<sub>2</sub> with Copper

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Fig. S1



Fig. S1. Electronic band structures of  $2H-MoS_2$  (a), and  $1T'-MoS_2$  (b) at PBE level. The horizontal dashed line at 0 eV denotes Fermi level.

Fig. S2



Fig. S2. Electronic band structures of Cu-adsorbed 2H-MoS<sub>2</sub> with the concentration of (a) 2%, (b) 4%, (c) 7.7%, (d) 14.3%, (e) 20%, and (f) 25% at PBE level. The horizontal dashed line at 0 eV denotes Fermi level.





Fig.S3. Partial density of states (PDOS) of Cu-adsorbed  $2H-MoS_2$  with the concentration of (a) 2%, (b) 4%, (c) 7.7%, (d) 14.3%, (e) 20%, and (f) 25% at PBE level. The vertical dashed line at 0 eV denotes the Fermi level.

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Fig.S4. Electronic band structures of Cu-adsorbed 1T-MoS<sub>2</sub> with the concentration of (a) 2%, (b) 4%, (c) 7.7%, (d) 14.3%, (e) 20%, and (f) 25% at PBE level. The horizontal dashed line at 0 eV denotes Fermi level.





Fig. S5. Partial density of states (PDOS) of Cu-adsorbed  $1T'-MoS_2$  with the concentration of (a) 2%, (b) 4%, (c) 7.7%, (d) 14.3%, (e) 20%, and (f) 25% at PBE level. The vertical dashed line at 0 eV denotes Fermi level.





Fig. S6. 3D distribution of charge density differences of (a) pristine  $2H-MoS_2$ , Cuadsorbed  $2H-MoS_2$  with the concentration of (b) 4% and (c) 14.3%, (d) pristine  $1T'-MoS_2$ , and Cu-adsorbed  $1T'-MoS_2$  with the concentration of (e) 4% and (f) 14.3%. The red color and green color represent the charge accumulation, and charge depletion, respectively.

Fig. S7.



Fig. S7. (a) Electronic band structures and (b) density of states (DOS) with partial density of states of Li of Li-adsorbed 2H-MoS<sub>2</sub> with the concentration of (a) 2% at PBE level. The dashed line at 0 eV denotes Fermi level.

Fig. S8



Fig. S8 Electronic band structures of  $2H-MoS_2$  (a), and  $1T'-MoS_2$  (b) calculated with HSE06 functional.

Fig. S9



Fig. S9 Electronic band structures of Cu-adsorbed 2H-MoS<sub>2</sub>with the concentration of (a) 7.7% and (b)14.3% and those of Cu-adsorbed 1T'-MoS<sub>2</sub> with the concentration of (c)7.7% and (d) 14.3% calculated with HSE06 functional.