Electronic Supplementary Material (ESI) for RSC Advances.

Theoretical study on the influence of a secondary metal on the Cu(110) surface with the presence of H_2O for methanol decomposition

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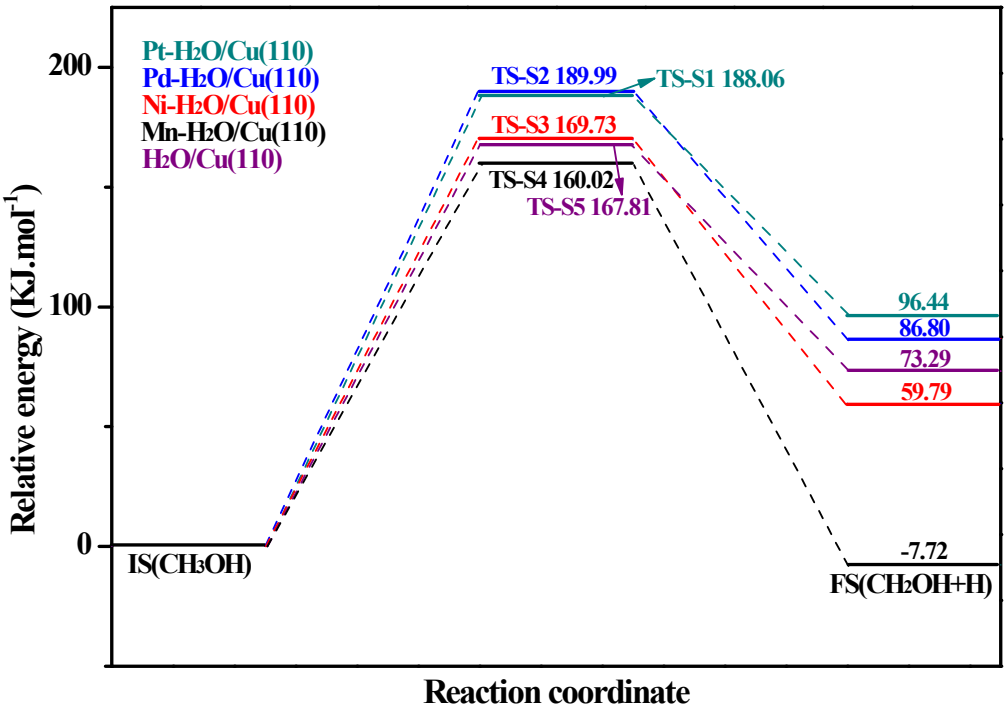
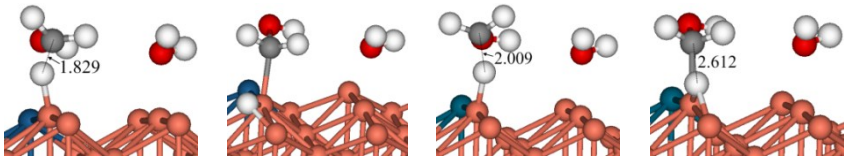
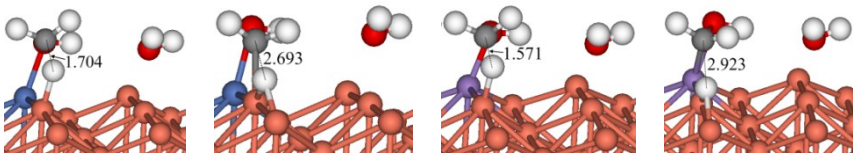
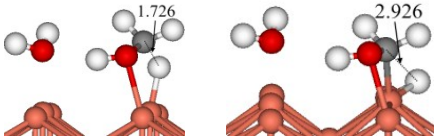




TS-S1 FS-S1(CH_2OH+H) TS-S2 FS-S2(CH_2OH+H)

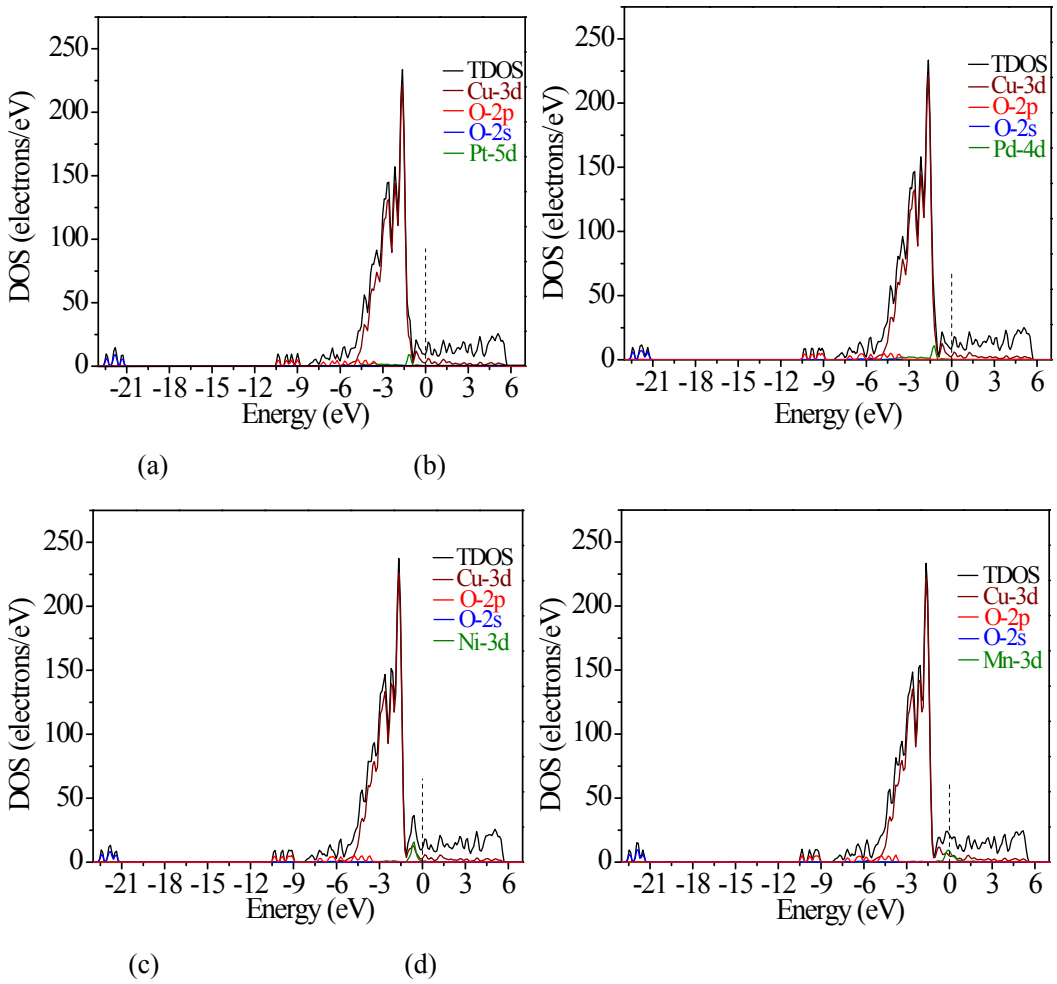


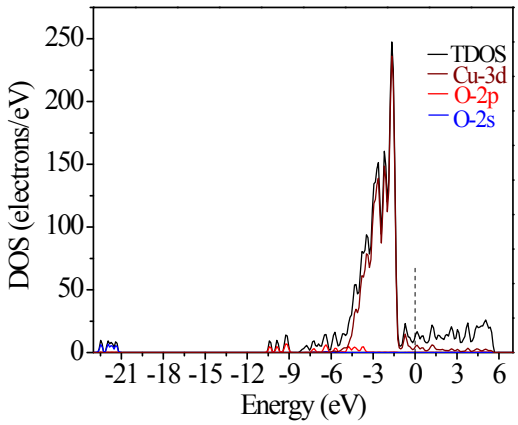
TS-S3 FS-S3(CH_2OH+H) TS-S4 FS-S4(CH_2OH+H)



TS-S5 FS-S5(CH_2OH+H)

Fig.S1. The potential energy profile for CH_3OH dehydrogenation to CH_2OH on the metal (Pt, Pd, Ni, Mn) doped and un-doped H_2O/Cu(110) surfaces with the corresponding structures of the TS, and FS. See Fig.2 for color coding.





(e)

Fig.S2. The calculated total and partial density of states of the metal doped H_2O/Cu(110) (Fig.S2-a~d)and un-doped H_2O/Cu(110) (Fig.S2-e), the Fermi energy is set to zero.