

Supplementary Information

Mechanistic insights to CO₂ reduction on Cu/ Mo loaded two-dimensional g-C₃N₄ (001)

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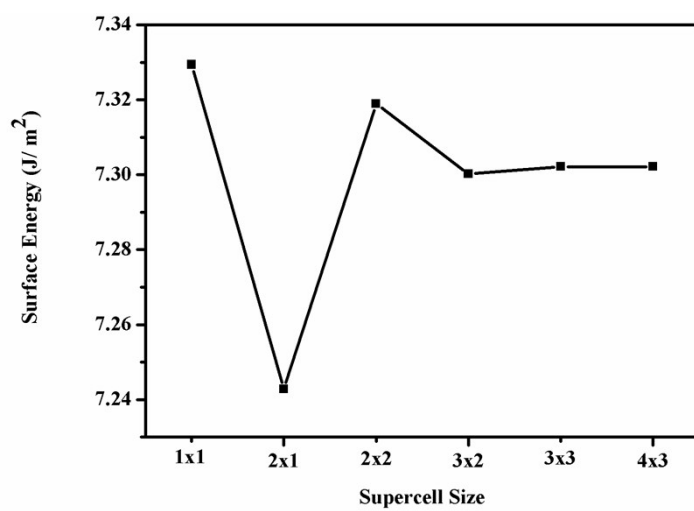


Fig. S1 Convergence tests of surface energies for pure-C₃N₄ (001) surface.

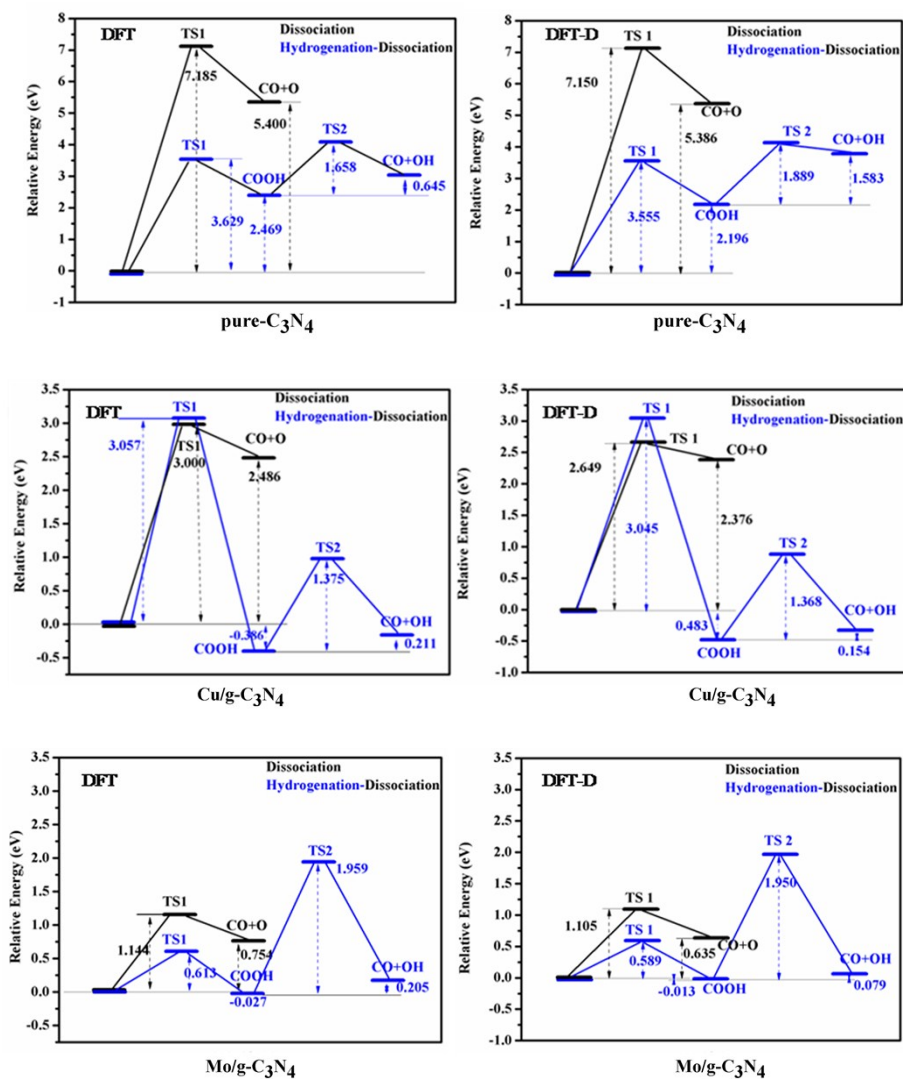


Fig. S2 Comparisons of two mechanisms of CO₂ activation on g-C₃N₄ (001), Cu/g-C₃N₄ (001) and Mo/g-C₃N₄ (001) with DFT and DFT-D method, respectively.