

Supporting Information

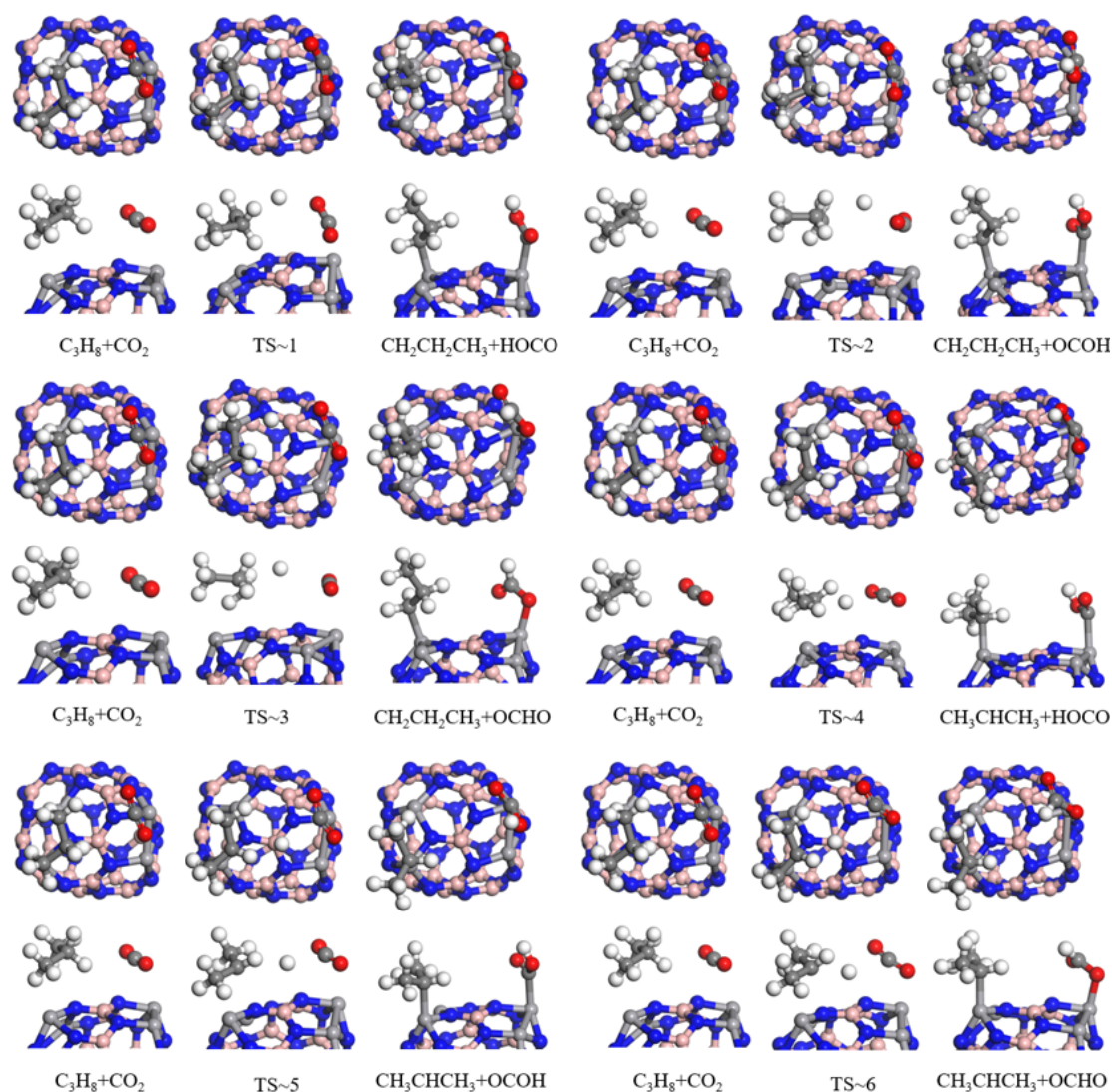


Figure S1. The most stable configuration of initial state (IS), transition state (TS) and final state (FS) in the initial oxidation reaction of C_3H_8 on the $V_4-B_{24}N_{28}$ surface are shown. Pink, blue, gray, red, and white respectively represent boron atoms, nitrogen atoms, carbon atoms, oxygen atoms, and hydrogen atoms, V atoms doped on the surface of the BN cage.

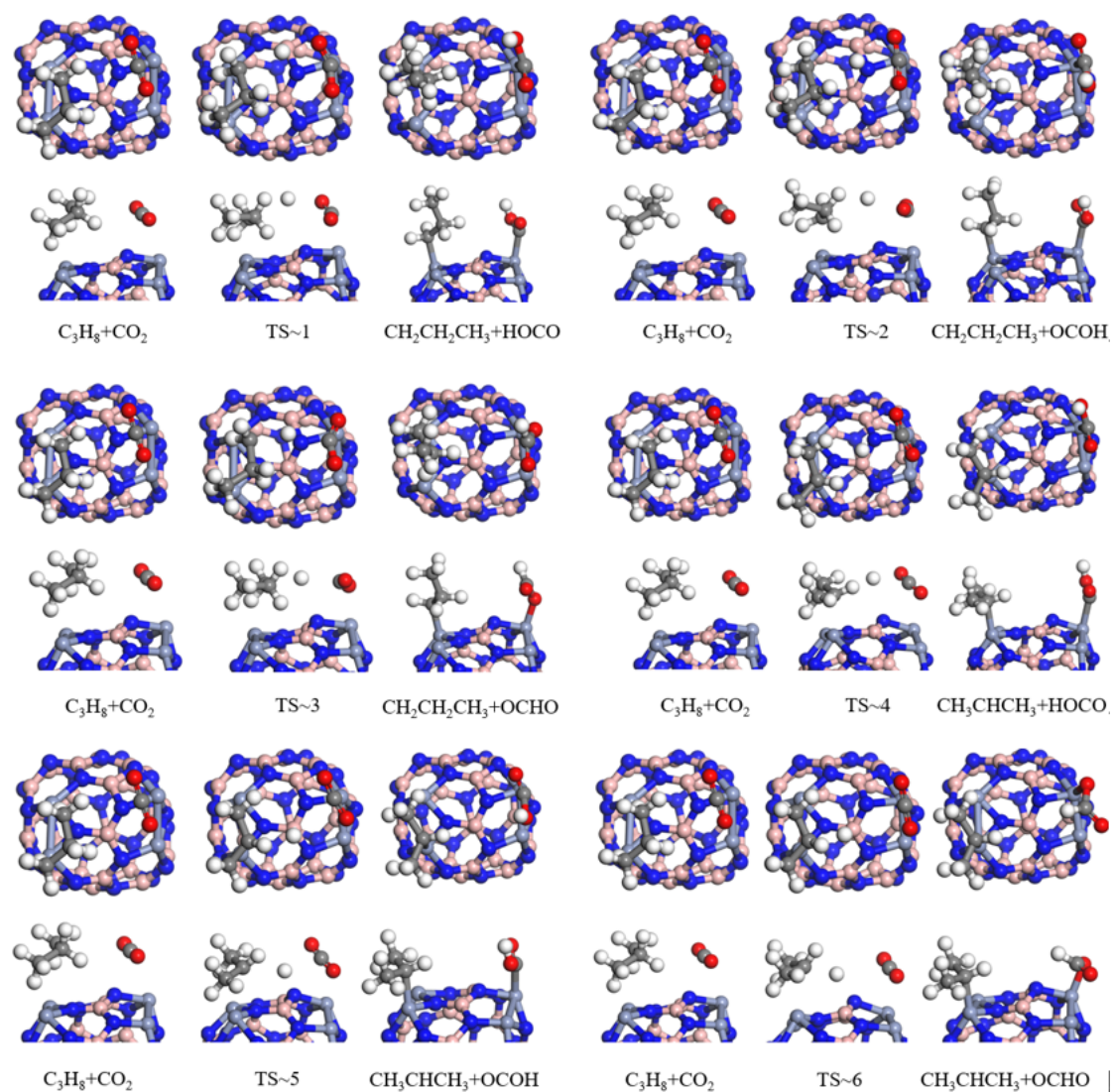


Figure S2. The most stable configuration of initial state (IS), transition state (TS) and final state (FS) in the initial oxidation reaction of C_3H_8 on the $Cr_4-B_{24}N_{28}$ surface are shown. Pink, blue, gray, red, and white respectively represent boron atoms, nitrogen atoms, carbon atoms, oxygen atoms, and hydrogen atoms, Cr atoms doped on the surface of the BN cage.

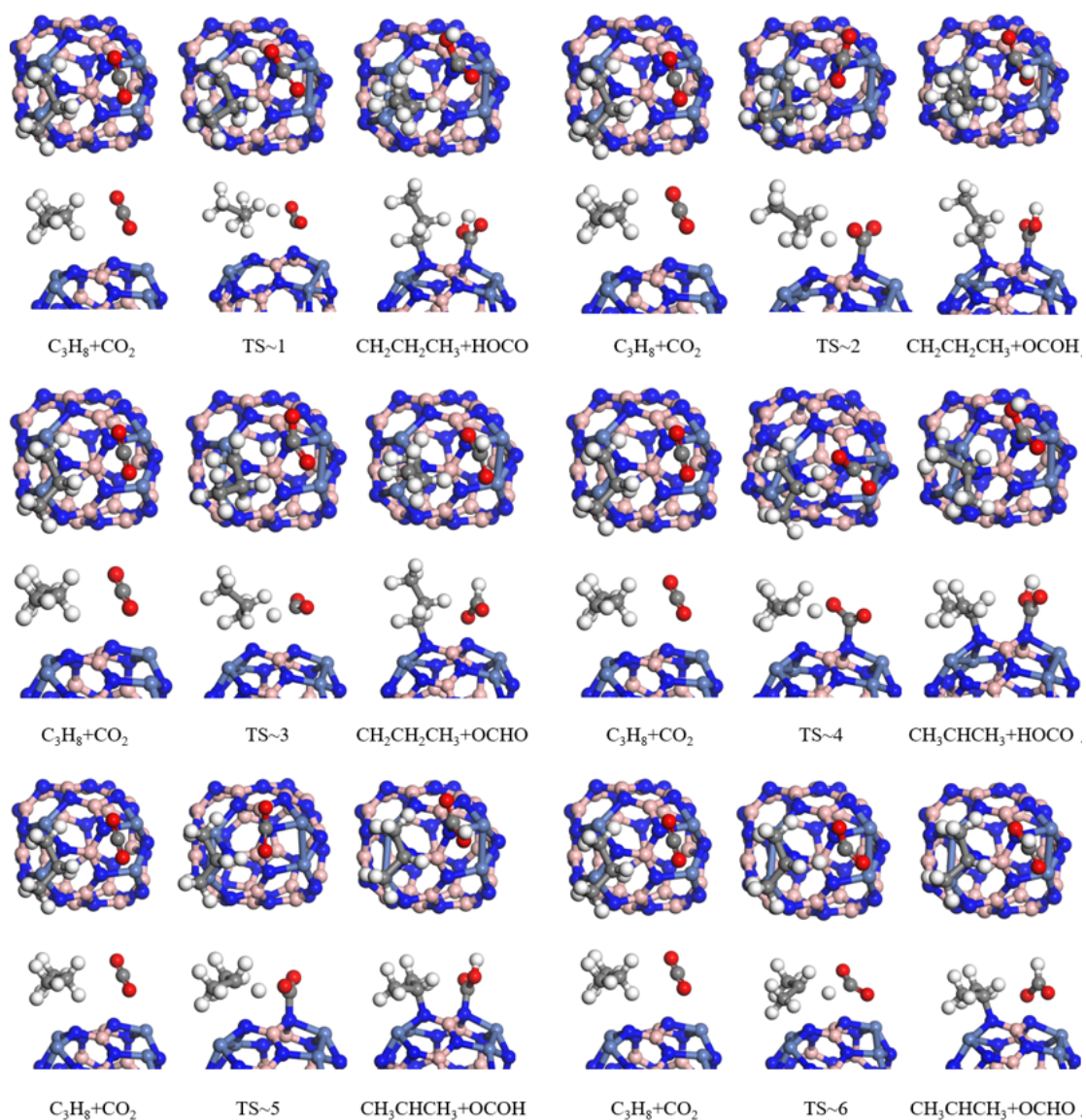


Figure S3. The most stable configuration of initial state (IS), transition state (TS) and final state (FS) in the initial oxidation reaction of C_3H_8 on the $Ni_4-B_{24}N_{28}$ surface are shown. Pink, blue, gray, red, and white respectively represent boron atoms, nitrogen atoms, carbon atoms, oxygen atoms, and hydrogen atoms, Ni atoms doped on the surface of the BN cage.

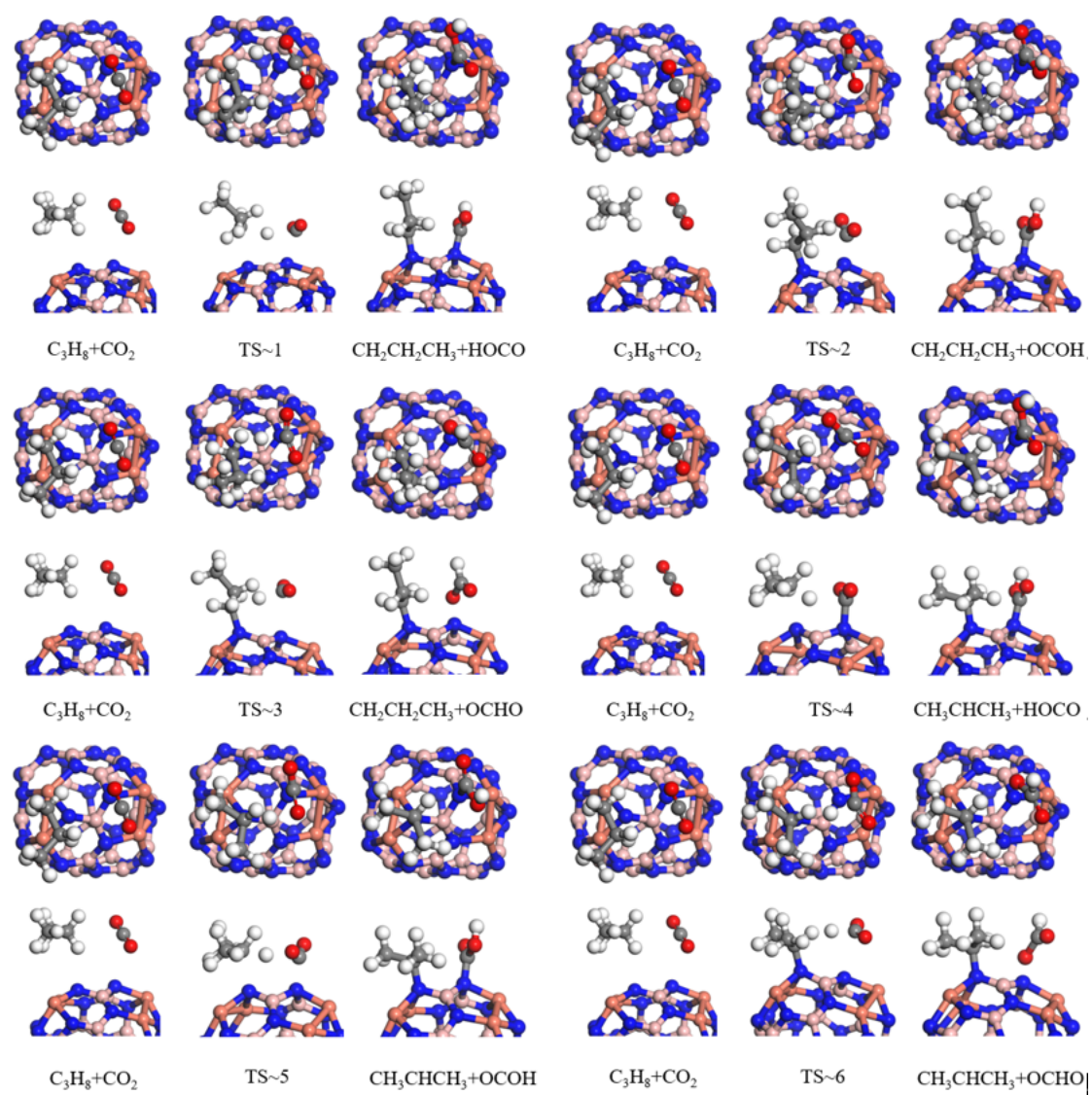


Figure S4. The most stable configuration of initial state (IS), transition state (TS) and final state (FS) in the initial oxidation reaction of C_3H_8 on the $Cu_4-B_{24}N_{28}$ surface are shown. Pink, blue, gray, red, and white respectively represent boron atoms, nitrogen atoms, carbon atoms, oxygen atoms, and hydrogen atoms, Cu atoms doped on the surface of the BN cage.

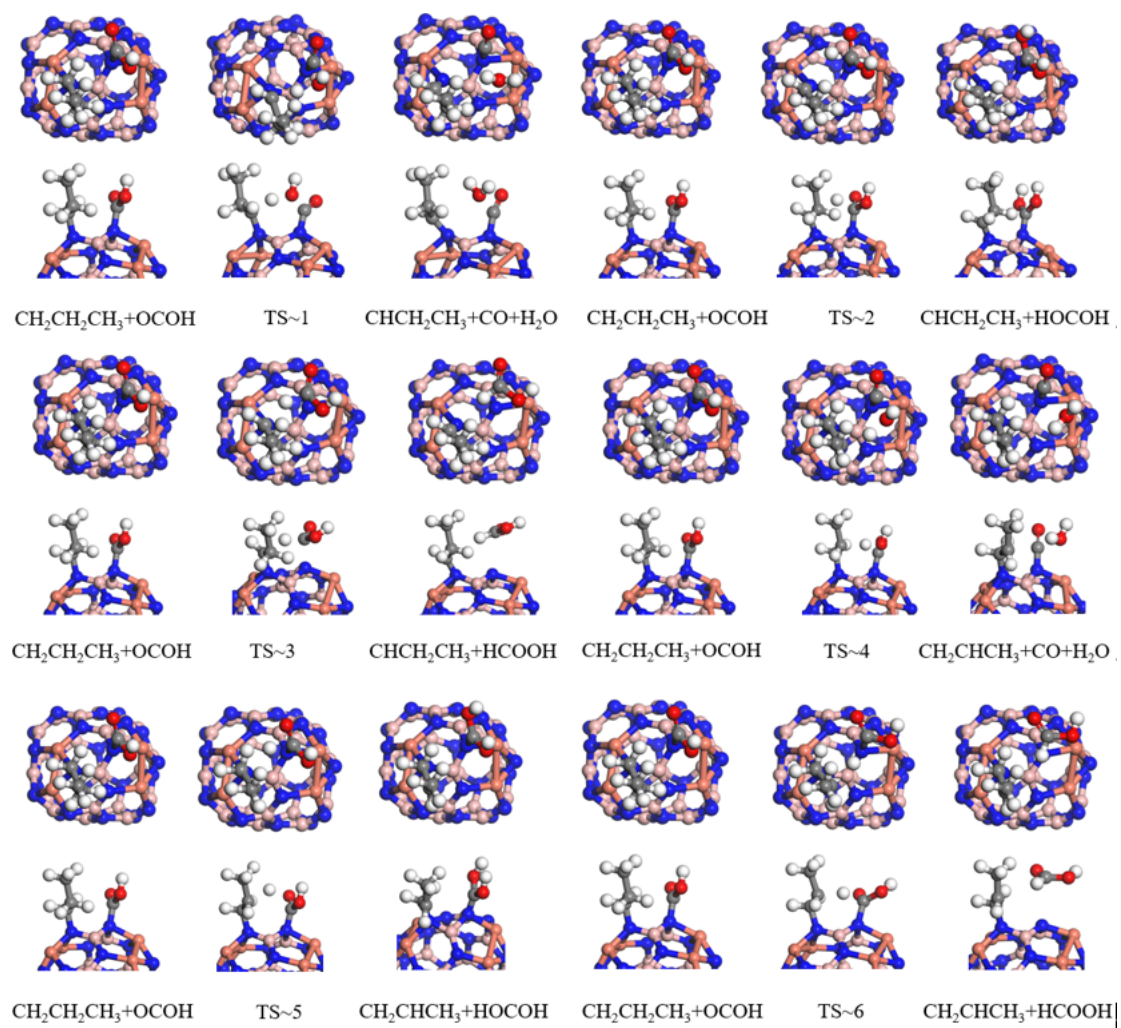


Figure S5. The most stable configuration of initial state (IS), transition state (TS) and final state (FS) in the oxidation reaction of propane by carbon dioxide to propylene and formic acid in the primary carbon dehydrogenation-O(2)-H path on the surface of $\text{Cu}_4\text{-B}_{24}\text{N}_{28}$.

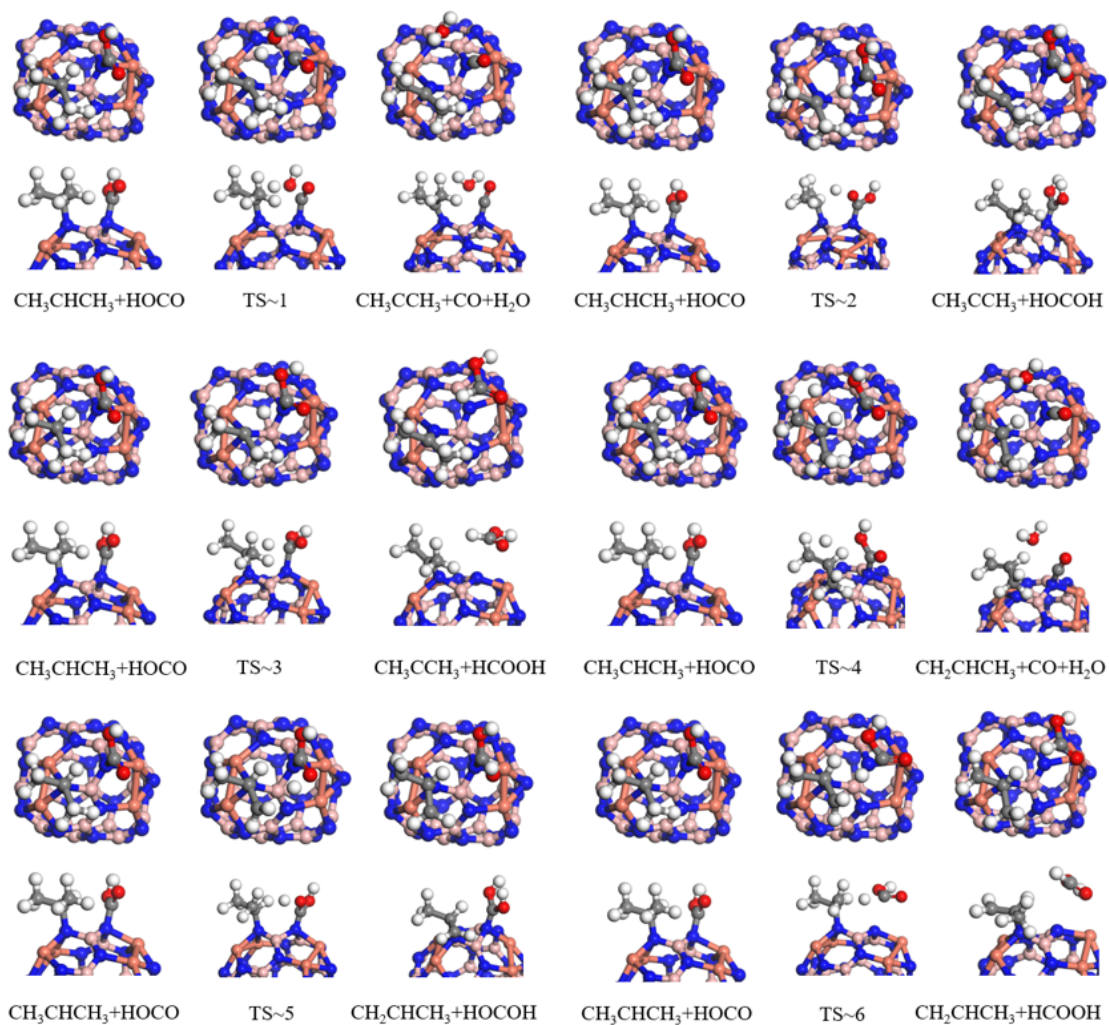


Figure S6. The most stable configuration of initial state (IS), transition state (TS) and final state (FS) in the oxidation reaction of propane by carbon dioxide to propylene and formic acid in the secondary carbon dehydrogenation-O(1)-H path on the surface of Cu₄-B₂₄N₂₈.

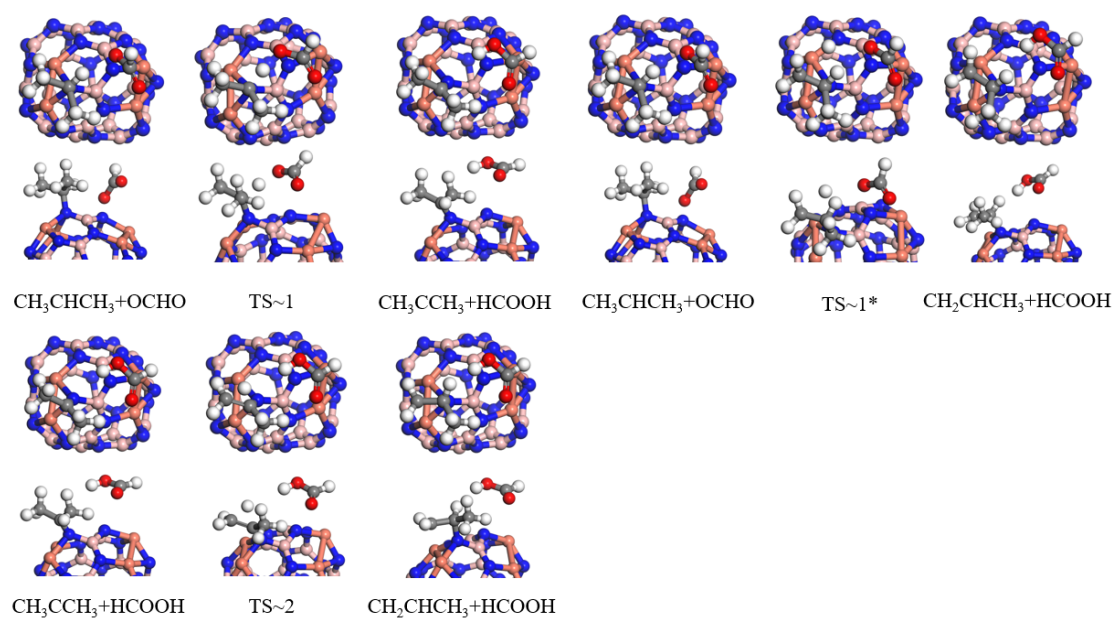


Figure S7. The most stable configuration of initial state (IS), transition state (TS) and final state (FS) in the oxidation reaction of propane by carbon dioxide to propylene and formic acid in the secondary carbon dehydrogenation-C-H path on the surface of Cu₄-B₂₄N₂₈.