Understanding the nature of NH_3-coordinated active sites and complete reaction schemes for NH_3-SCR using Cu-SAPO-34 catalysts

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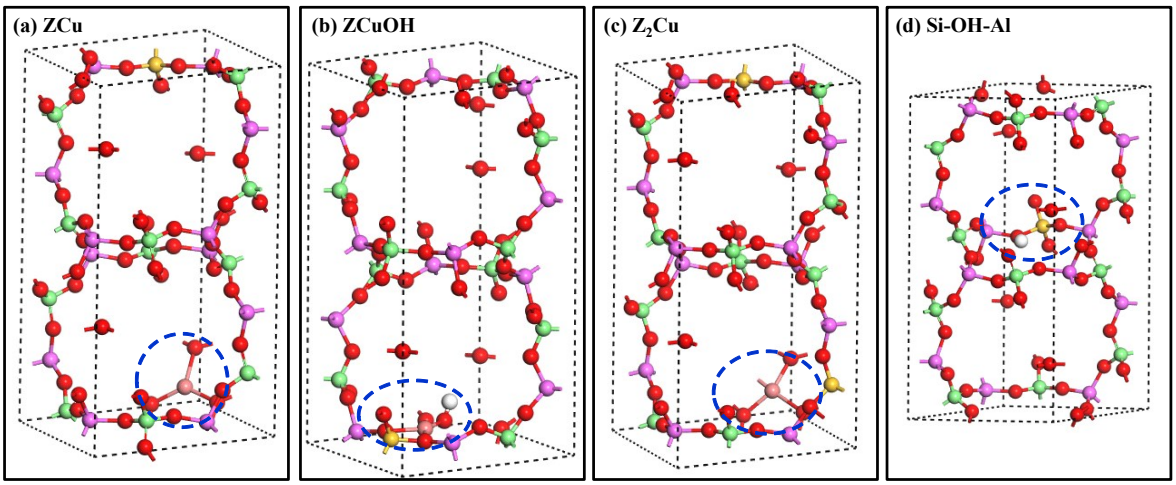

Fig. S1 Optimized periodic structures of Cu-SAPO-34 with (a) ZCu, (b) ZCuOH and (c) Z_2Cu species, and (d) H-SAPO-34 configuration with Si-OH-Al in 2 × 1 × 1 supercells. Green, red, purple, yellow, orange, and white balls represent P, O, Al, Si, Cu, and H atoms, respectively. This assignment will be applied throughout the paper.

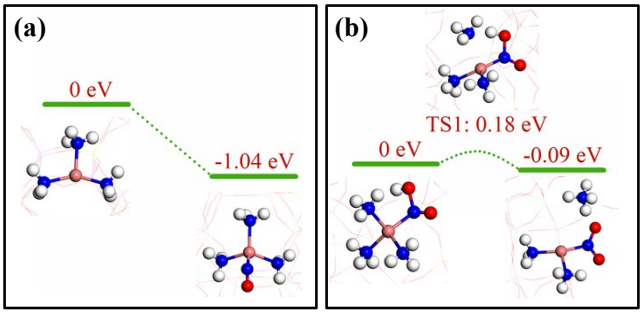

Fig. S2 Energy profiles for (a) NO adsorption on Z_2Cu-$3NH_3$ complex, and (b) NH_4NO_2 formation on ZCuOH-$3NH_3$ complex. Blue balls represent N atoms, and this assignment will be applied throughout the paper.

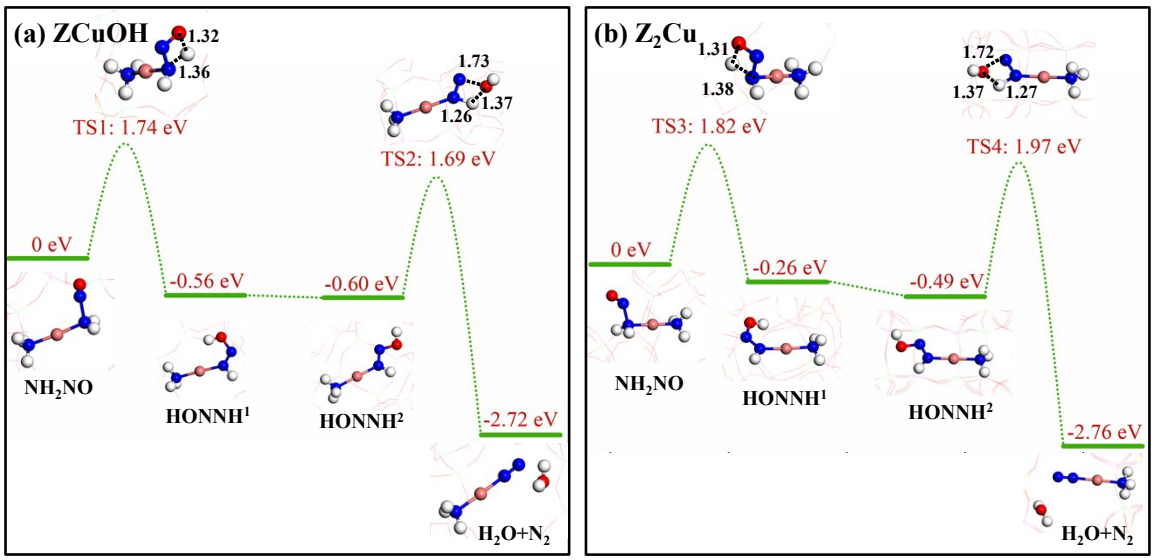

Fig. S3 Energy profiles for NH_2NO decomposition processes on (a) ZCuOH-$2NH_3$ complex and (b) Z_2Cu-$2NH_3$ complex.

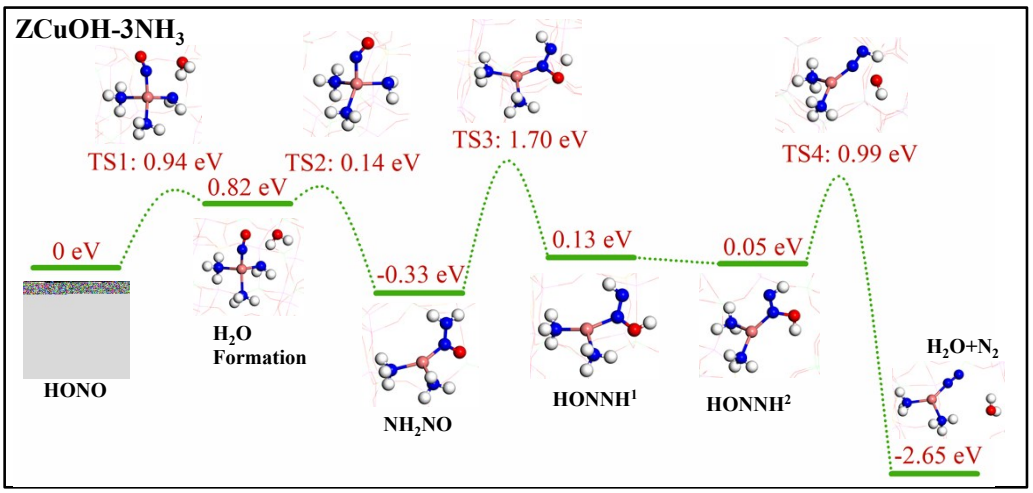

Fig. S4 Energy profiles for NH_2NO formation and decomposition processes on ZCuOH-$3NH_3$.

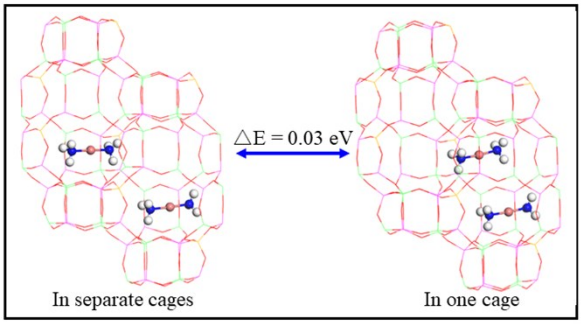

Fig. S5 Structures of two ZCu-$2NH_3$ complexes in separate cages and one cage, and energy difference of them.

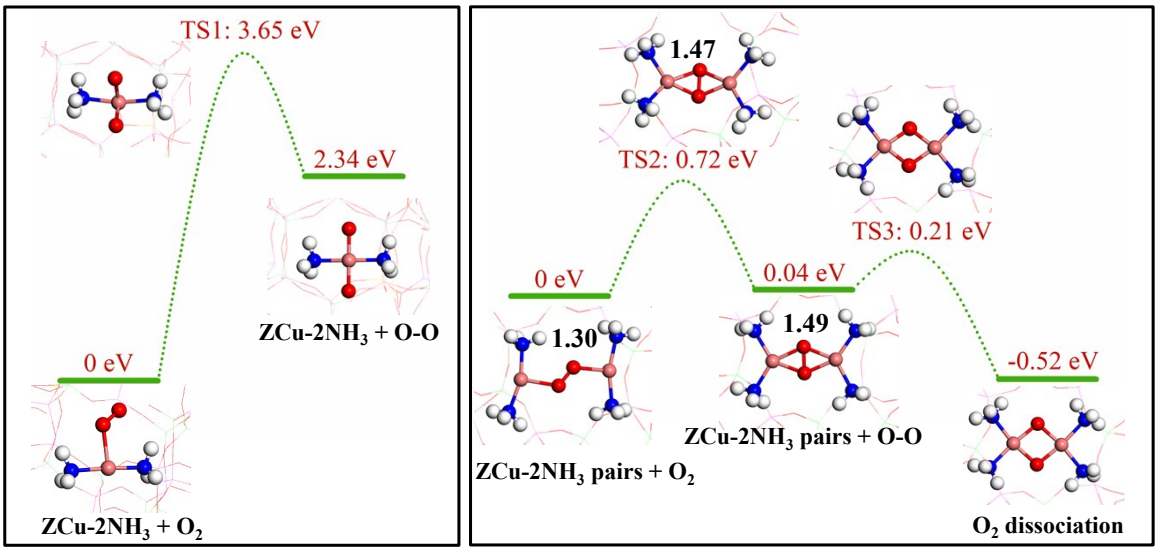

Fig. S6 Energy profiles for the dissociation of O_2 on (a) a single ZCu-2NH_3 site and (b) a pair of ZCu-2NH_3 site in SAPO-34.

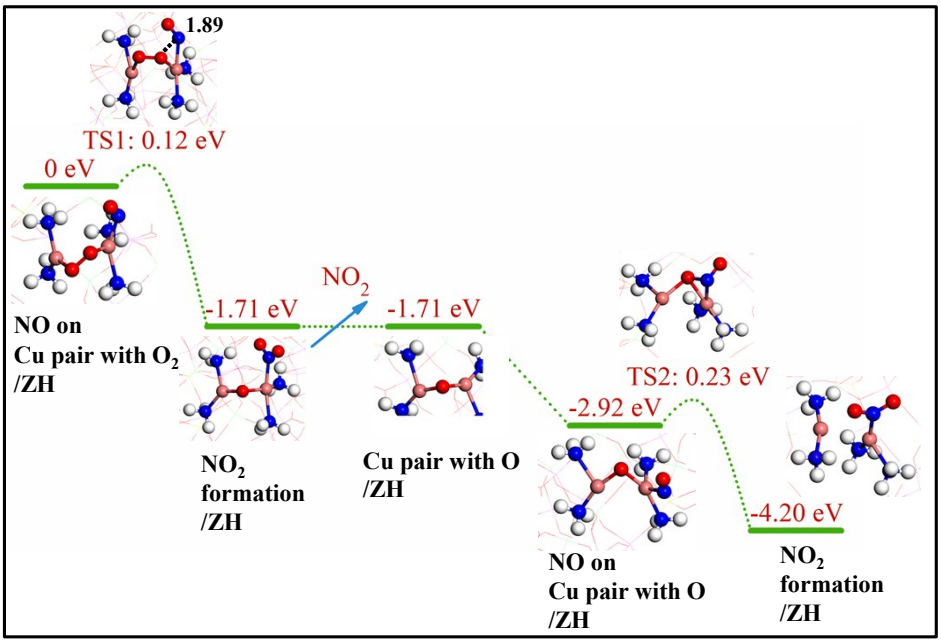

Fig. S7 Energy profiles for the re-oxidation process to produce Z_2Cu-2NH_3 complex. Atomic distances are in Å.