

Supplementary Information (SI)

Promotional mechanism of enhanced denitration activity with Cu modification in Ce/TiO₂-ZrO₂ catalyst for low temperature NH₃-SCR system

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Fig. S1 Optimized structures of the intermediates and the transition states for NH_3 dehydrogenation reaction on the Cu atoms. The bond lengths are given in Å.

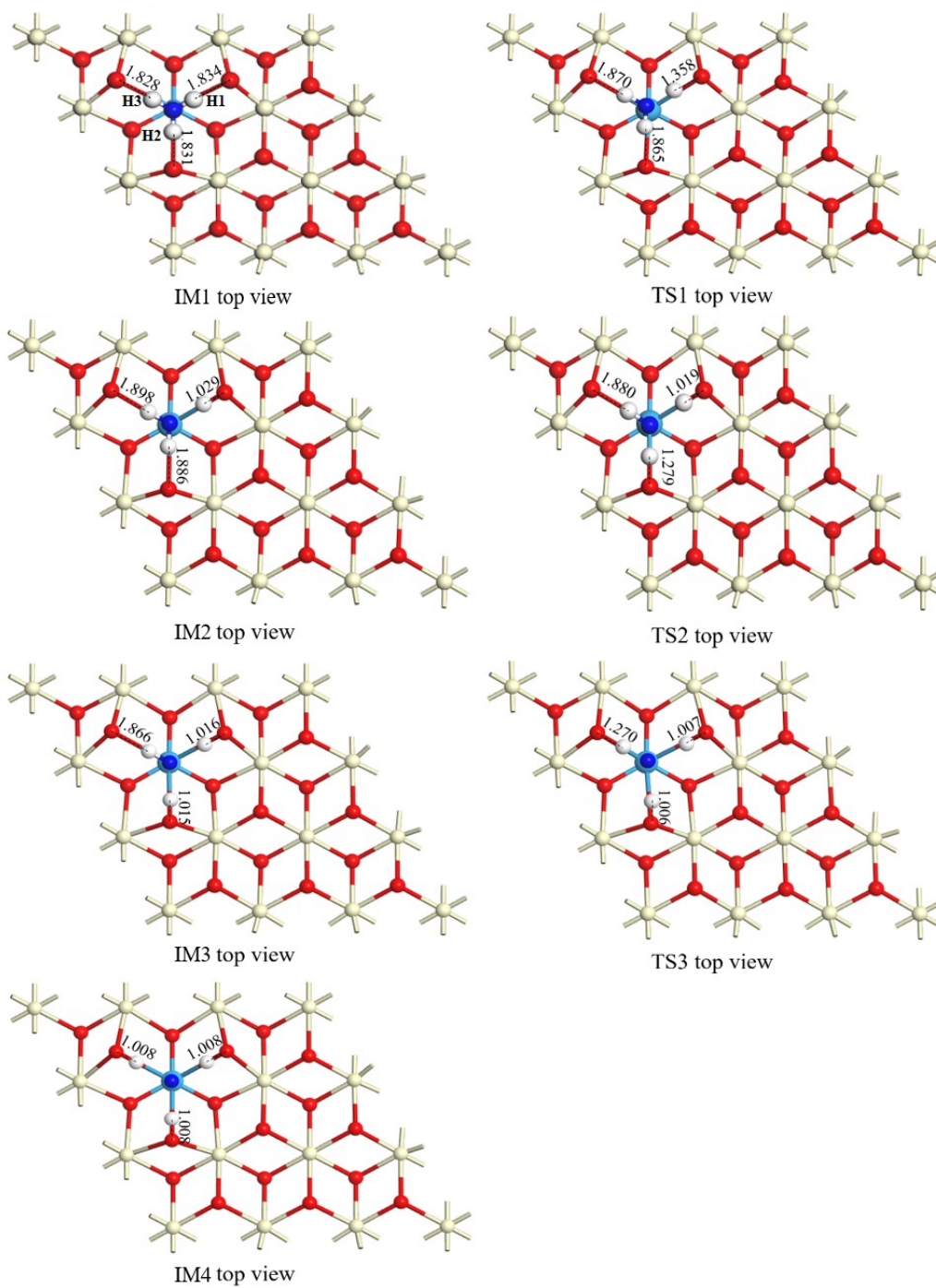


Fig. S2 Optimized structures (top view) of NO adsorptions on (a) Cu-NH₂, (b) Cu-NH, (c) Cu-N, (d) NH₂-Cu-OH, (e) NH₂-Cu-O. The bond lengths are given in Å.

