Supplementary Information

Reaction Pathway and Kinetic Origin of Low-Temperature NH_3-SCR over a Mn–Cu Dual-Atom Catalyst: A DFT Study

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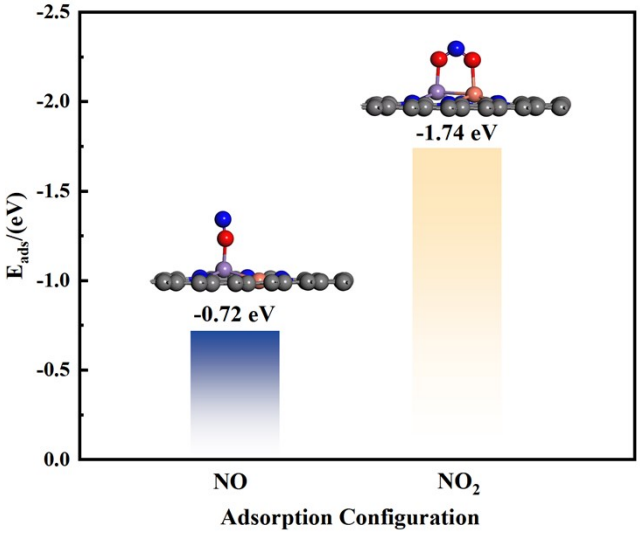

Figure S1 Adsorption energies and configurations of NO and NO_2 on the Mn–Cu/NG catalyst in the O-bound configuration.

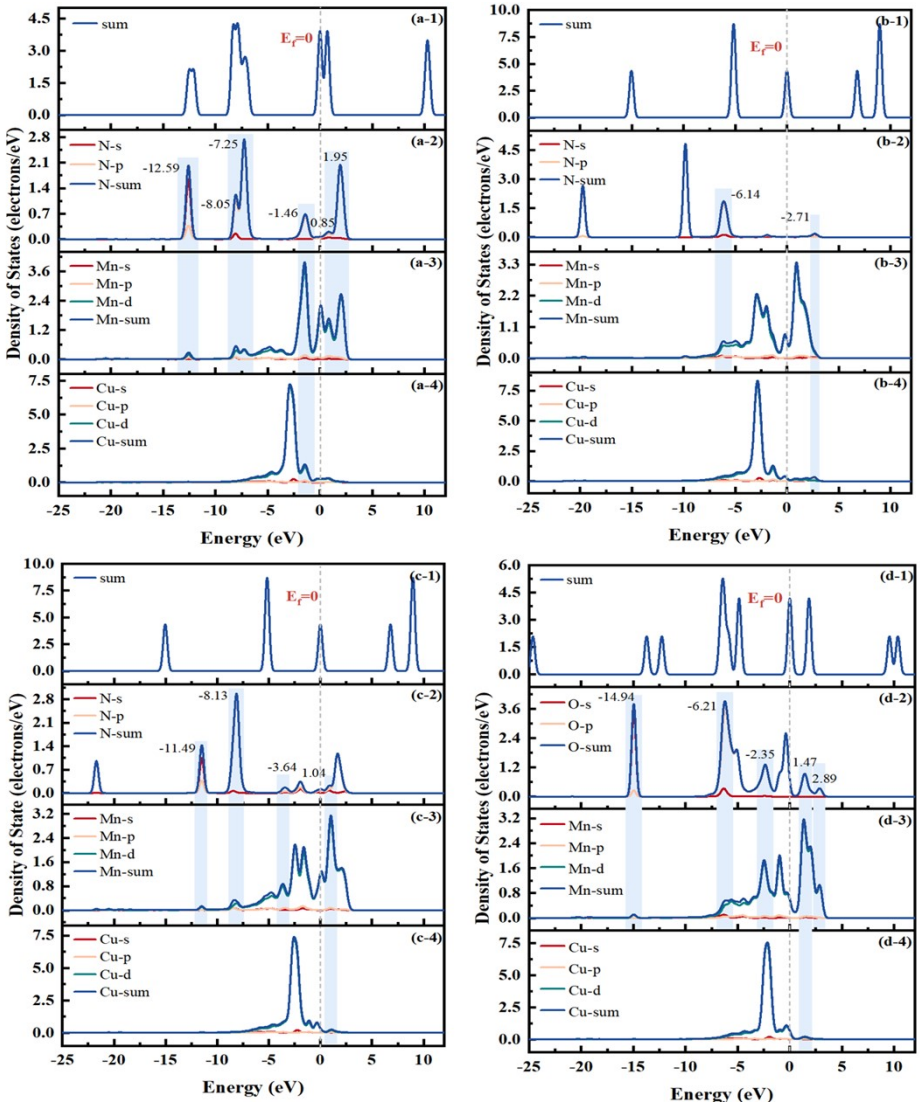

Figure S2 Projected density of states (PDOS) of (a) NO, (b) NH_3, (c)NO_2, and (d) O_2 adsorbed on the Mn–Cu/NG catalyst surface.

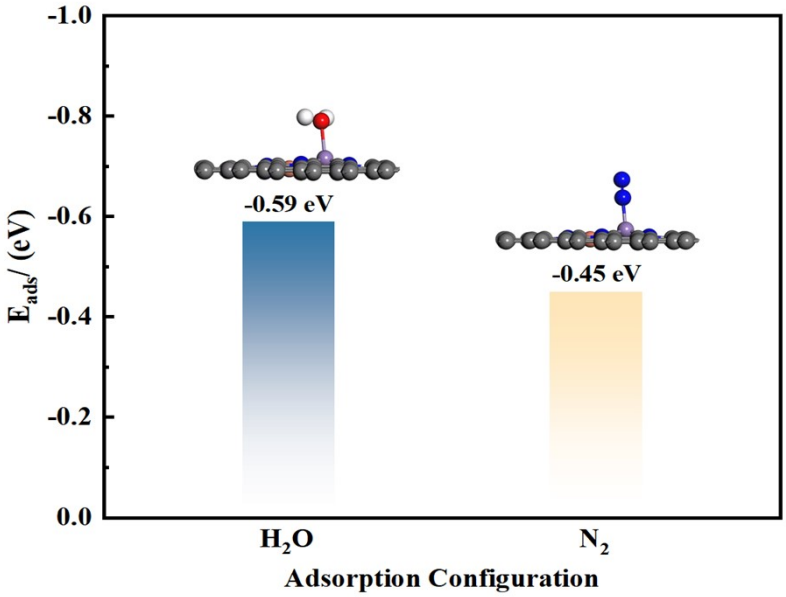

Figure S3 Adsorption energies and configurations of H_2O and N_2 molecules on the Mn–Cu/NG catalyst.

Table S1 Proposed complete reaction mechanism for catalytic dehydrogenation reaction pathway in NH_3-SCR reaction on the Mn–Cu/NG.

Pathway	Reaction mechanism
Path 4 and Path 5	$*NO_2+*H\rightarrow*ONOH$
	$*ONOH + NH_3\rightarrow*NH_2NO+H_2O$
	$* NH_2NO\rightarrow*NHNOH$
	$* NHNOH\rightarrow*N_2+H_2O$
	$*N_2H\rightarrow*H+*N_2$

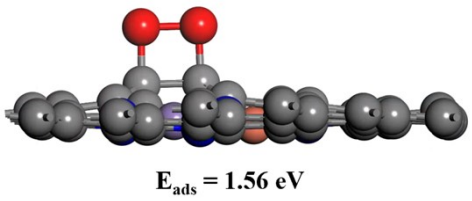

Figure S4 Adsorption configuration and adsorption energy of O_2 on nitrogen-doped graphene.

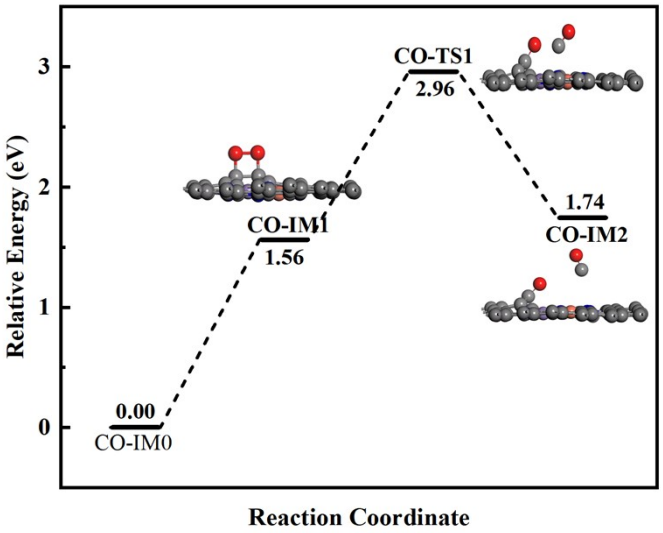

Figure S5 Energy profile for CO formation from the reaction between O_2 and nitrogen-doped graphene.

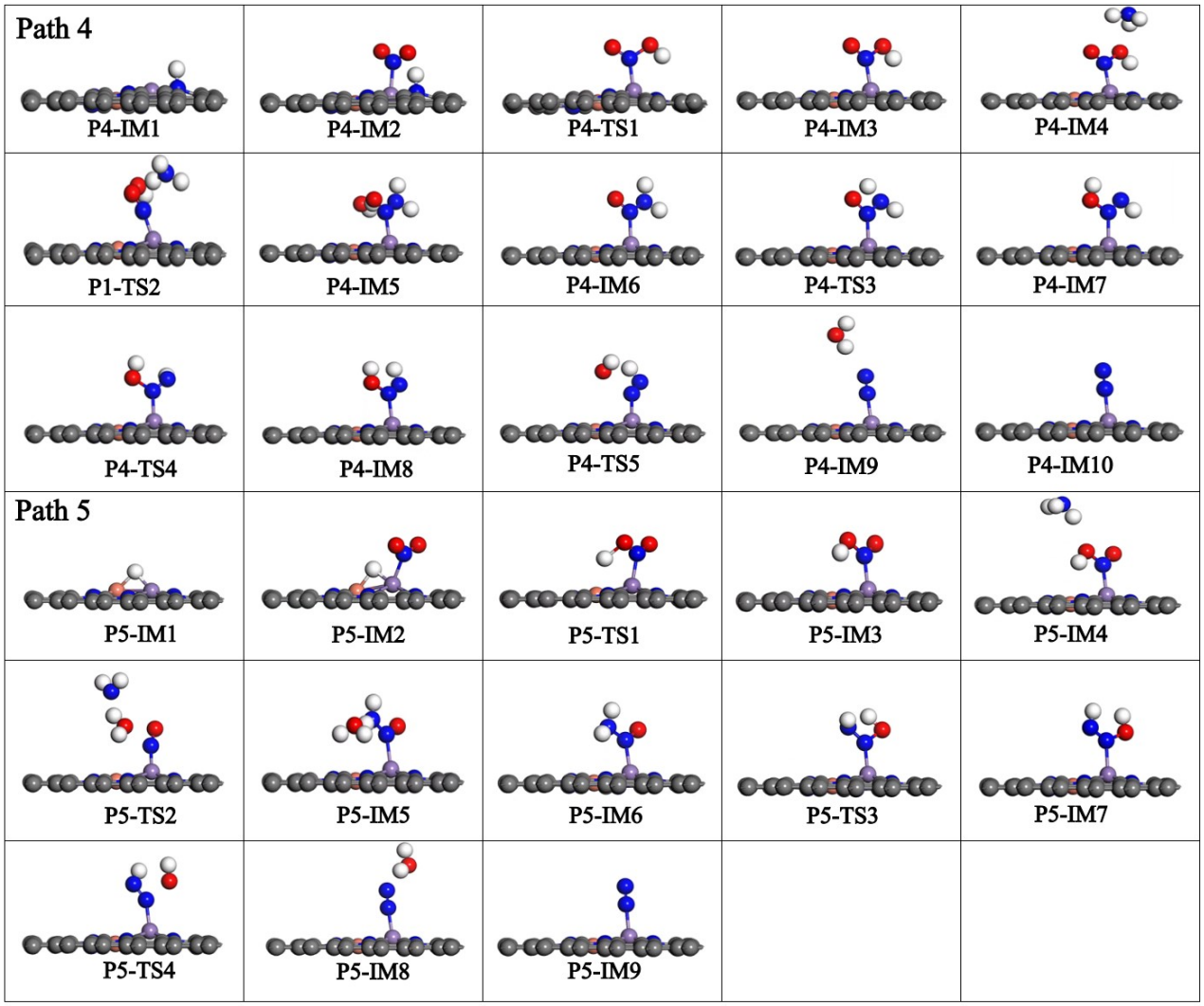

Figure S6 The configurations of initial states, transition states, intermediates, and final states for catalytic dehydrogenation reaction pathway in NH_3-SCR reaction on the Mn–Cu/NG.

Table S2 Proposed complete reaction mechanism for NH_3-SCR over the Mn–Cu/NG catalyst

Pathway	Rate-determining step	Energy barrier (eV)
Path 1	P1-IM9 → P1-TS5	1.83
Path 2	P2-IM4 → P2-TS4	2.22
Path 3	P3-IM1 → P3-TS1	1.23

Table S3 Activation energies for NO reduction over various catalysts.

Catalysts	Activation energy (eV)	Reference
Cu-SAPO-34	1.50	1
W-Doped CeO_2	1.36	2
$Cu_5Nd_{0.5}$@X zeolite	2.16	3
Fe_2O_3/MnO_2	1.11	4
Fe/γ-Al_2O_3	1.74	5
$CrMn_{1.5}O_4$	1.42	6
Fe-$CeCO_3F$	2.44	7
Mn–Cu/NG	0.80	This work

References

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