Supplementary Information

Density functional study on the CO oxidation reaction mechanism on MnN_2-doped graphene

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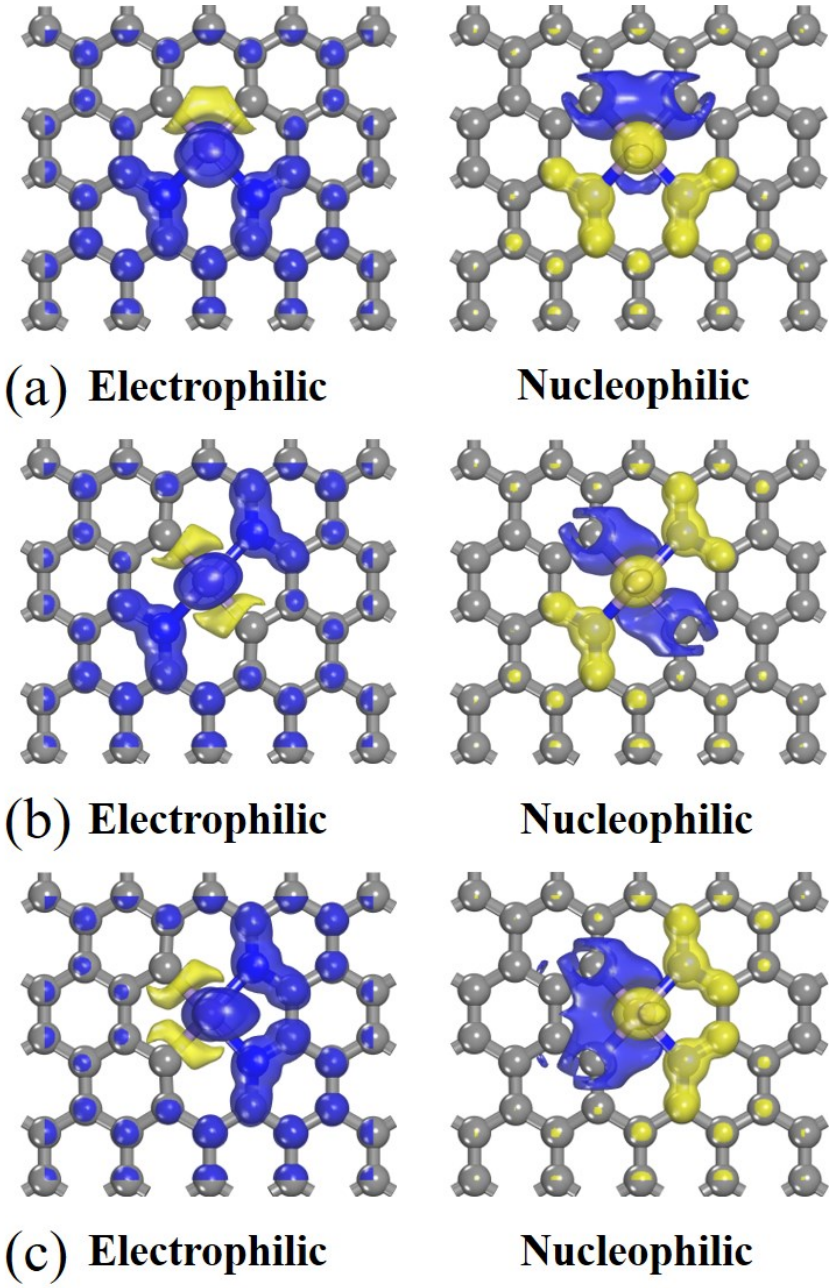

Fig. S1 The Fukui function of (a) MnN_2C_2-hex, (b) MnN_2C_2-opp and (c) MnN_2C_2-pen, the isosurface value is 3 e/Å^3.

Table S1 The adsorption energy (eV) of gas on MnN_2C_2.

	MnN_2C_2-hex	MnN_2C_2-opp	MnN_2C_2-pen
CO_2	−0.292	−0.270	−0.260
CO	−1.448	−1.318	−1.424
O_2	−1.778	−1.975	−1.655

$CO+O_2$	−2.490	−2.283	−2.327
2CO	−2.423	−2.524	−2.395

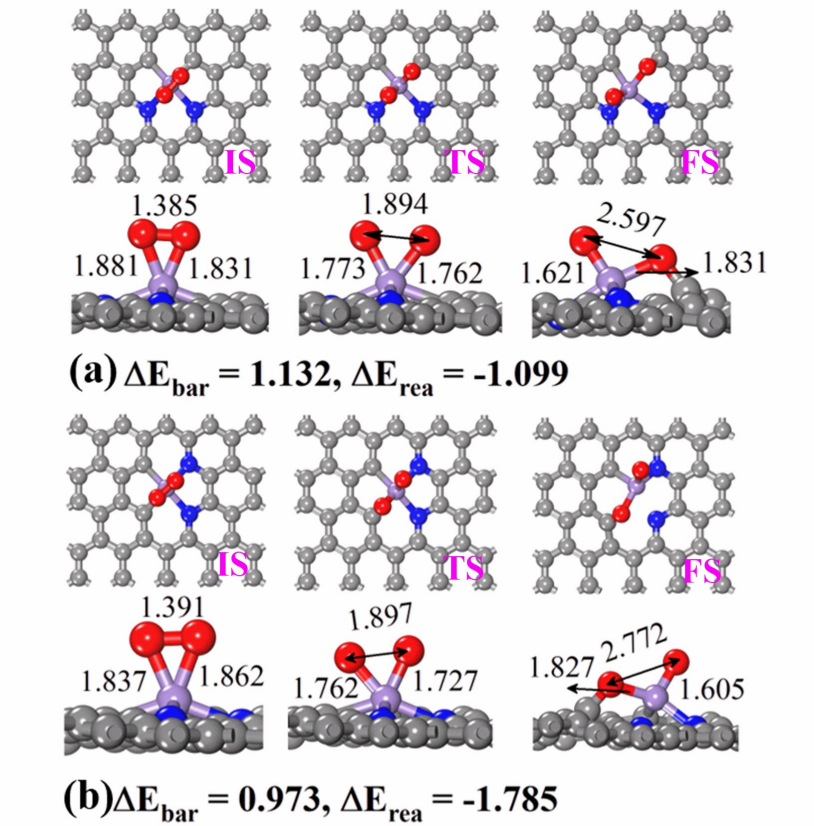

Fig. S2 Structure of O_2 decomposition reaction on (a) MnN_2C_2-hex and (b) MnN_2C_2-pen. ΔE_{bar} represents reaction barrier (eV) and ΔE_{rea} represents reaction energy (eV).

Table S2 The energy barriers and reaction energies of CO oxidation along the ER mechanism. ΔE_{bar} represents reaction barrier (eV) and ΔE_{rea} represents reaction energy (eV).

Model	Reaction	ΔE_{bar}(eV)	ΔE_{rea}(eV)
MnN_2C_2-hex	$CO_3 \rightarrow O+CO_2$	0.704	−0.193
	$O_2+CO \rightarrow O+CO_2$	1.101	−3.620
MnN_2C_2-opp	$CO_3 \rightarrow O+CO_2$	0.961	−0.126

	O_2+CO→O+CO_2	0.544	−3.611
MnN_2C_2-pen	CO_3→O+CO_2	1.110	−0.334
	O_2+CO→O+CO_2	0.950	−3.761

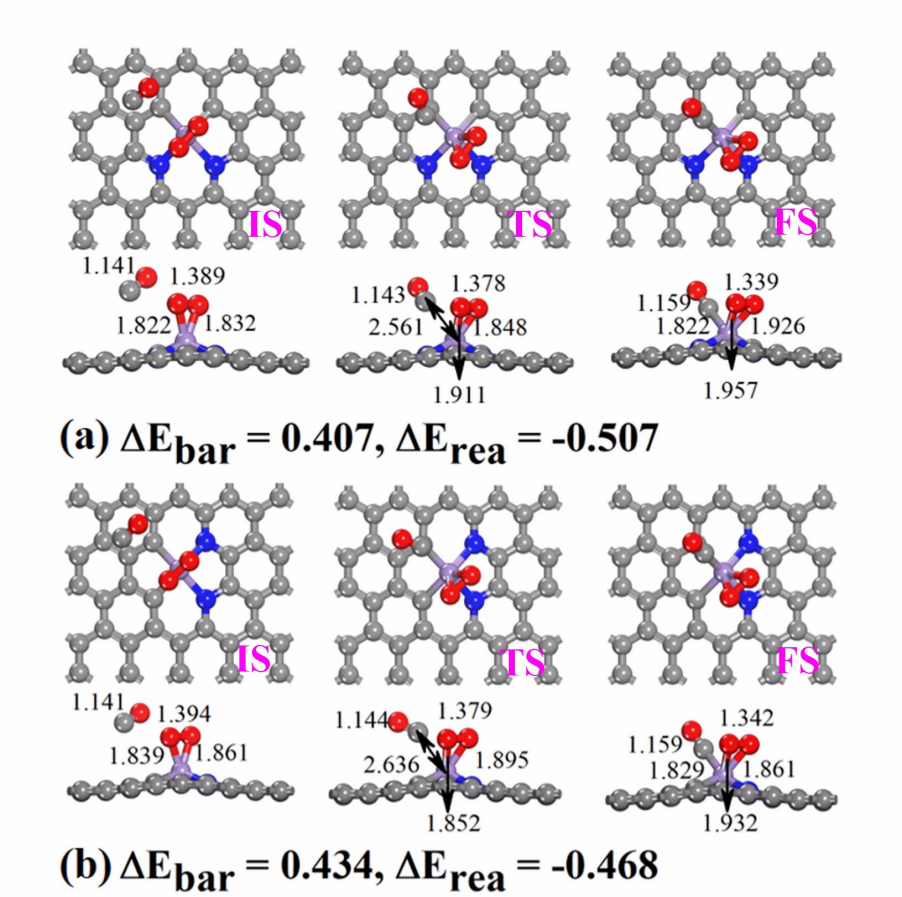

Fig. S3 Structure of the CO + *O_2 → *CO + *O_2 reaction on (a) MnN_2C_2-hex and (b) MnN_2C_2-pen. ΔE_{bar} represents reaction barrier (eV) and ΔE_{rea} represents reaction energy (eV).

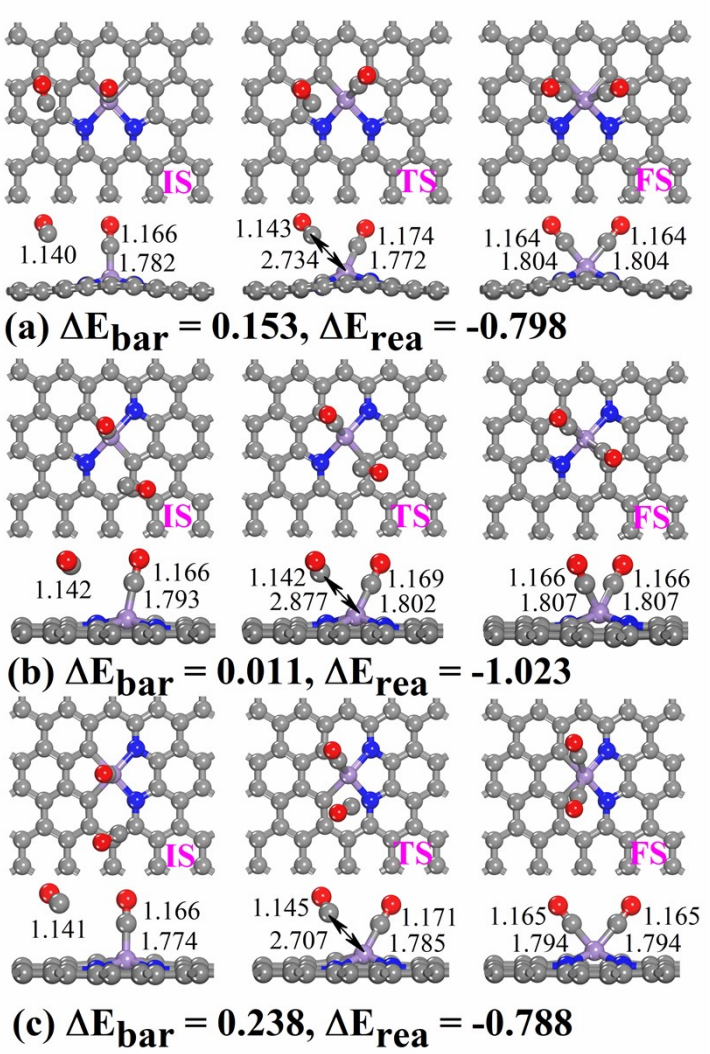

Fig. S4 The second CO is adsorbed on the Mn atom to form structure of two CO co-adsorption on (a) MnN_2C_2-hex, (b) MnN_2C_2-opp and (c) MnN_2C_2-pen. ΔE_{bar} represents reaction barrier (eV) and ΔE_{rea} represents reaction energy (eV).

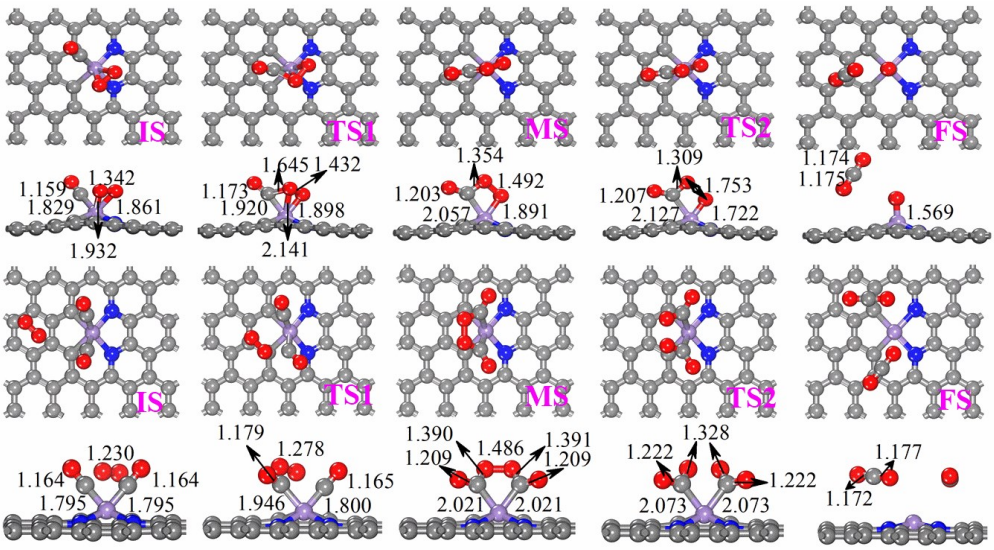

Fig. S5 Structure of the oxidation of CO on MnN_2C_2-pen along the LH and TER mechanisms.

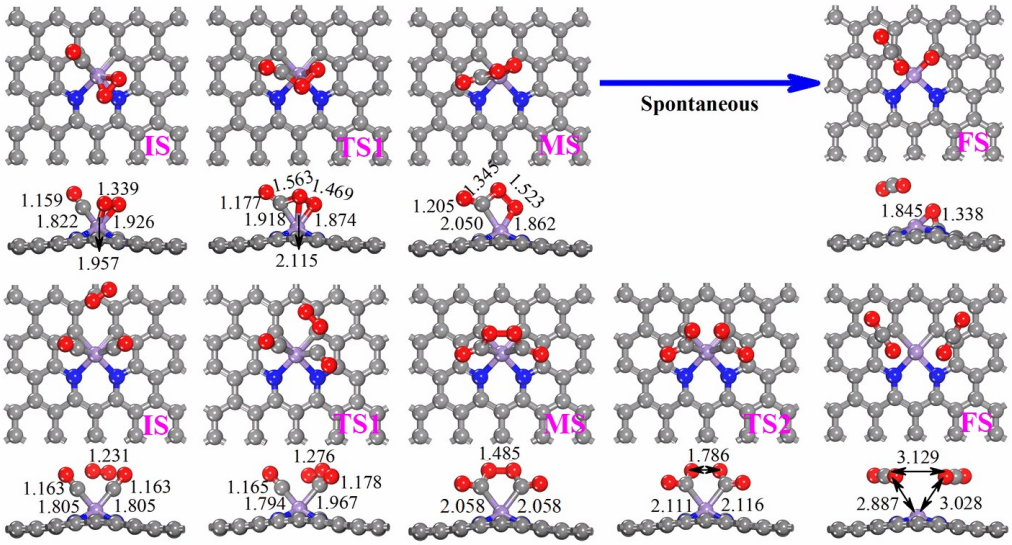

Fig. S6 Structure of the oxidation of CO on MnN_2C_2-hex along the LH and TER mechanisms.

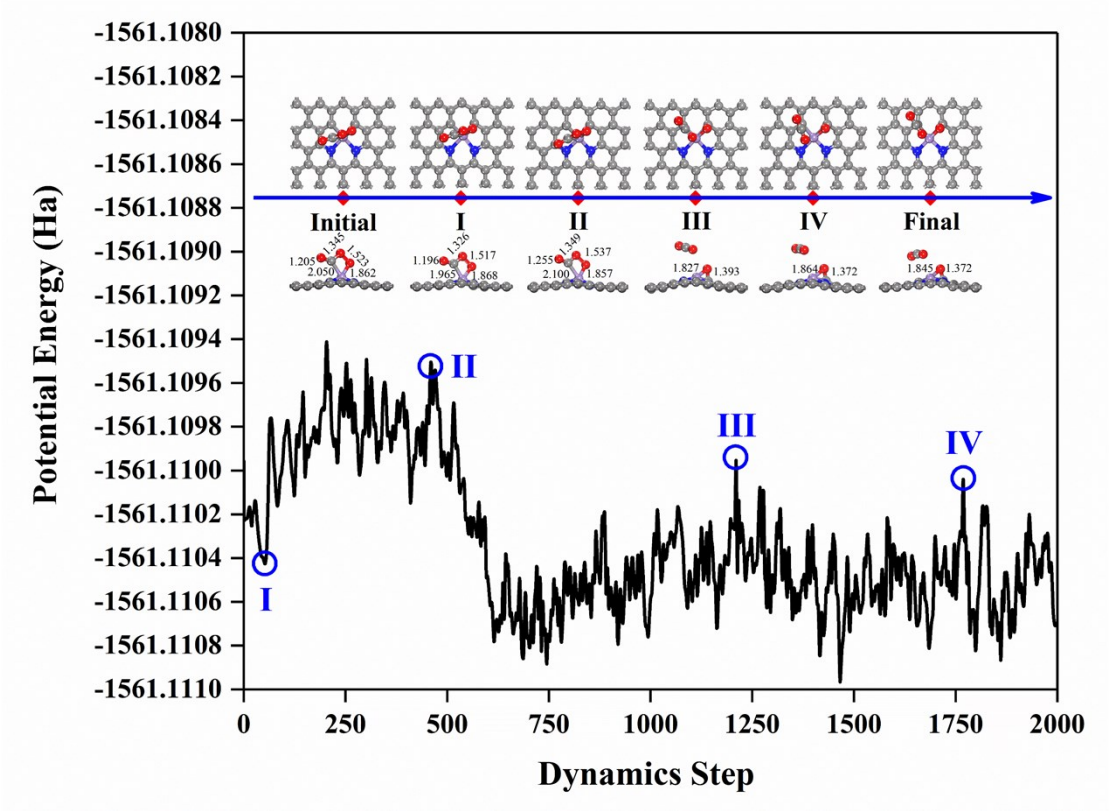

Fig. S7 Molecular dynamics trajectory of intermediate product OCOO spontaneously decomposes into O and CO_2 on MnN_2C_2-hex at 350 K with snapshots of intermediates at different times.