Supplementary Information

Catalytic oxidation mechanisms of carbon monoxide over single- and double-vacancy Mn-embedded graphene

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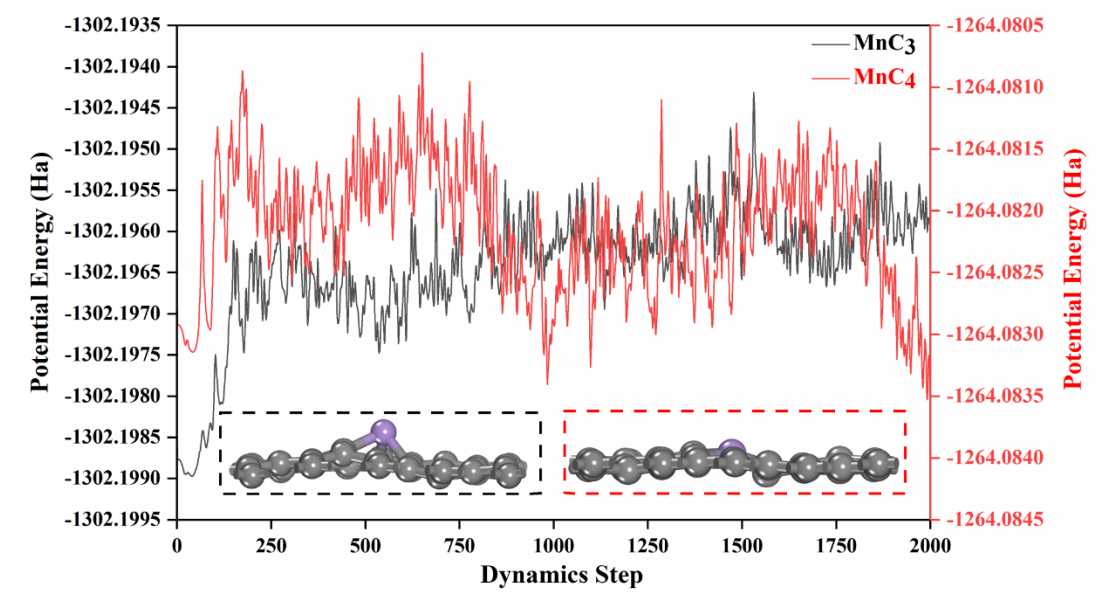

Fig. S1. The final structure (MnC_3 and MnC_4) from dynamics simulation at 1000 K and potential energy change.

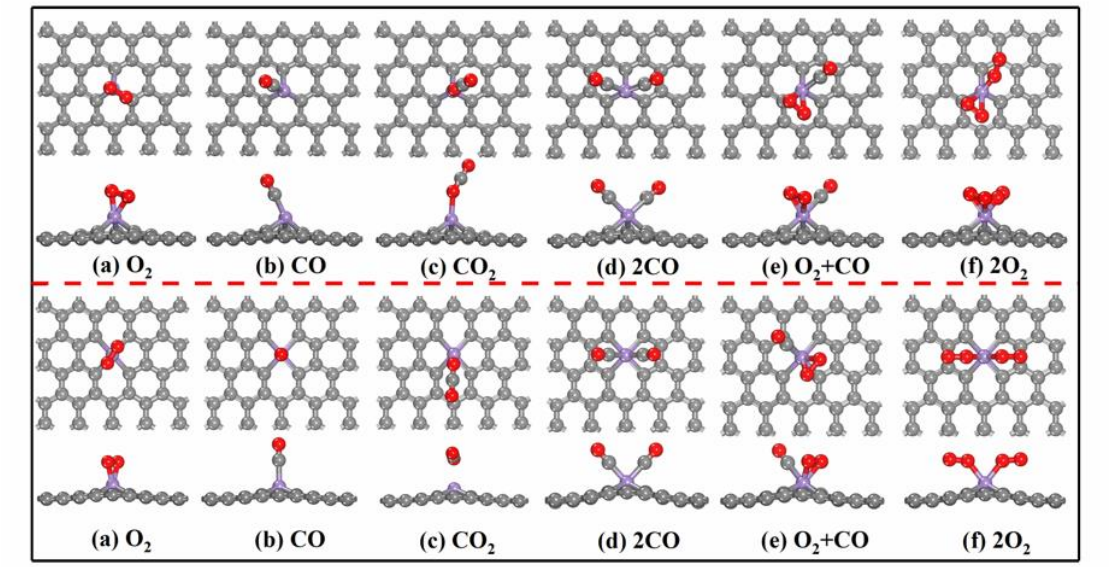

Fig. S2. The most stable configuration of O_2, CO, CO_2 and bimolecular co-adsorption on MnC_3 and MnC_4.

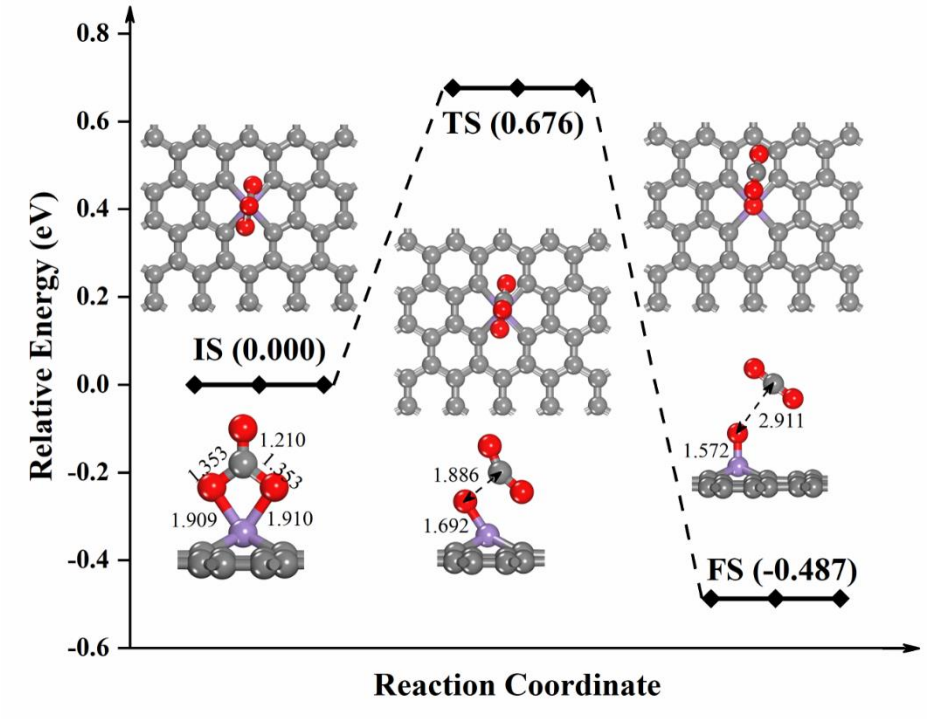

Fig. S3. OCOO is cracked into O and CO_2.

Table S1 The energy barrier of RDS (reaction mechanism) and second CO_2 generation of MnC_3 and MnC_4, * represents the substrate at room temperature (298.15 K), -- represents the CO oxidation process has not been studied (or the reaction is not RDS and the effect of temperature has not been studied), the unit is eV.

Models	ER	LH	O+CO→CO_2	TER
MnC_3	0.832	0.829	--	--
*MnC_3	0.835	0.761	--	--
MnC_4	--	0.568	0.851	1.011
*MnC_4	--	0.538	0.767	1.083