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Supplementary Information for

Revealing the crystal facet effect on N_2O formation during the NH_3-SCR over α-MnO_2 catalysts

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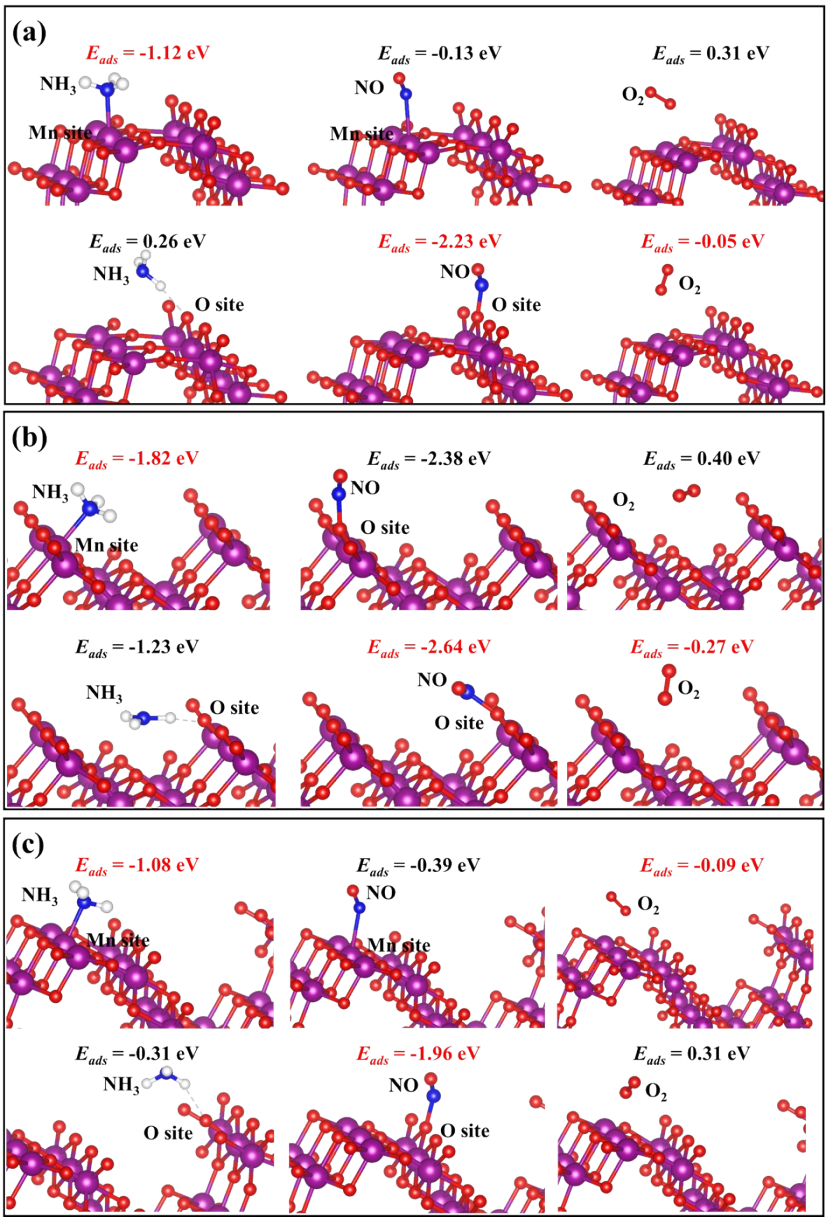

Fig. S1 Adsorption configurations of NH_3, NO and O_2 molecules on (a) α-MnO_2 (100); (b) α-MnO_2 (110); (c) α-MnO_2 (310). Purple, red, dark blue and white circles denote Mn, O, N and H atoms respectively.

Table S1 Reaction rate constant (k) of each elementary reaction on α-MnO_2 under different temperatures.

Facets	Reaction rate constants (k, s^{-1})	Temperature (K)				
		350	375	400	425	450
(100)	k (R1)	2.79×10^{-7}	7.37×10^{-6}	1.33×10^{-4}	1.75×10^{-3}	1.76×10^{-2}
	k (R2)	4.56×10^{4}	1.73×10^{5}	5.59×10^{5}	1.57×10^{6}	3.95×10^{6}
	k (R3)	2.09×10^{11}	2.47×10^{11}	2.87×10^{11}	3.28×10^{11}	3.69×10^{11}
(110)	k (R1)	3.59×10^{1}	1.75×10^{2}	7.05×10^{2}	2.41×10^{3}	7.19×10^{3}
	k (R2)	1.18×10^{-2}	9.09×10^{-2}	5.36×10^{-1}	2.54	10.03
	k (R3)	3.59×10^{1}	1.82×10^{2}	7.57×10^{2}	2.66×10^{3}	8.13×10^{3}
(310)	k (R1)	2.47×10^{9}	3.72×10^{9}	5.33×10^{9}	7.32×10^{9}	9.71×10^{9}
	k (R2)	2.15×10^{-1}	1.65	9.89	48.05	1.96×10^{2}
	k (R3)	1.55×10^{-4}	2.09×10^{-3}	2.06×10^{-2}	2.16×10^{-1}	9.41×10^{-1}