Supplementary Information (SI) for Physical Chemistry Chemical Physics.

Electronic regulation of first-coordination-shell environments in Mn-based single-atom sites for electrochemical NO reduction: A density functional theory study

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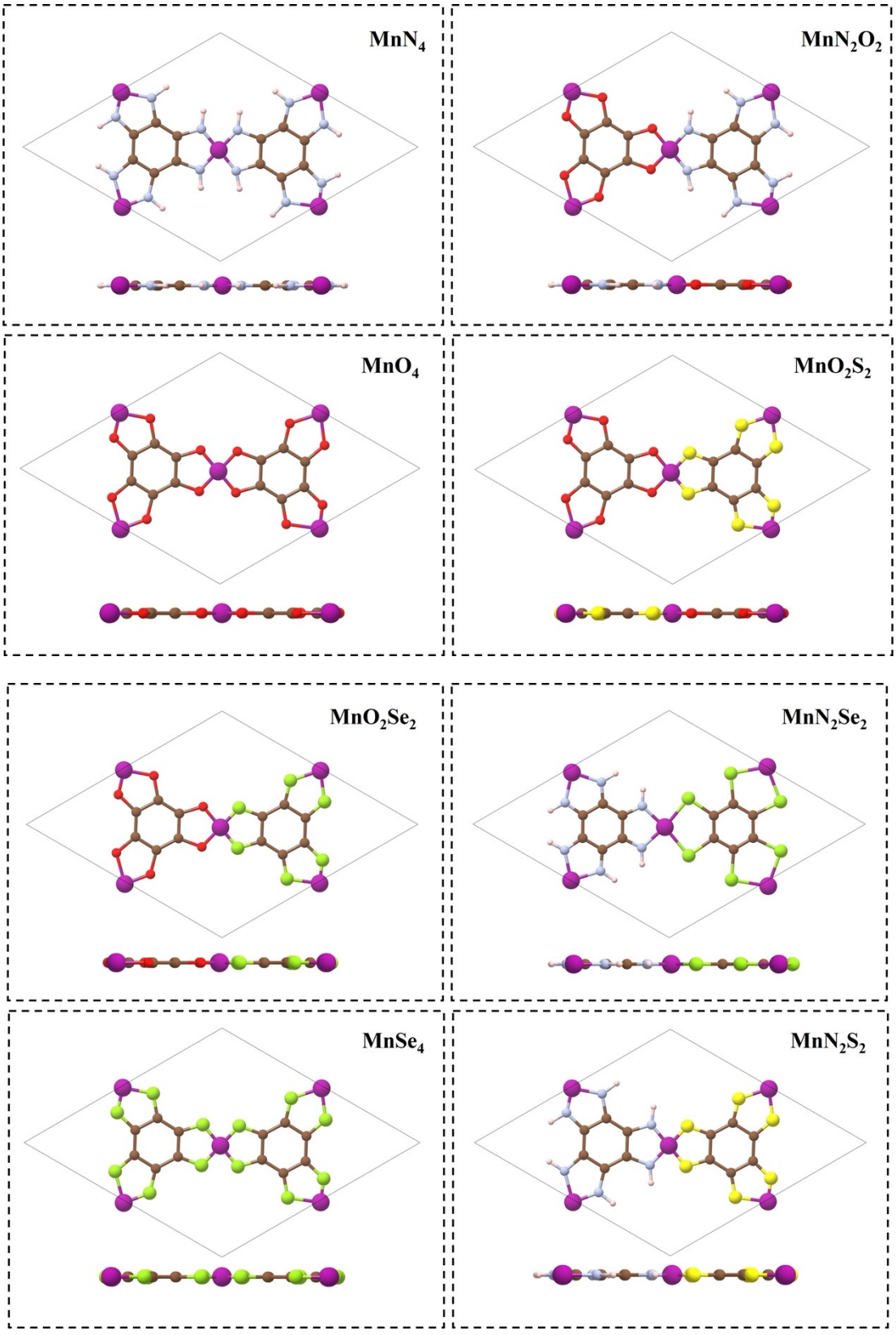
MnN4
MnN2O2
MnO4
MnO2S2
MnO2Se2
MnN2Se2
MnSe4
MnN2S2

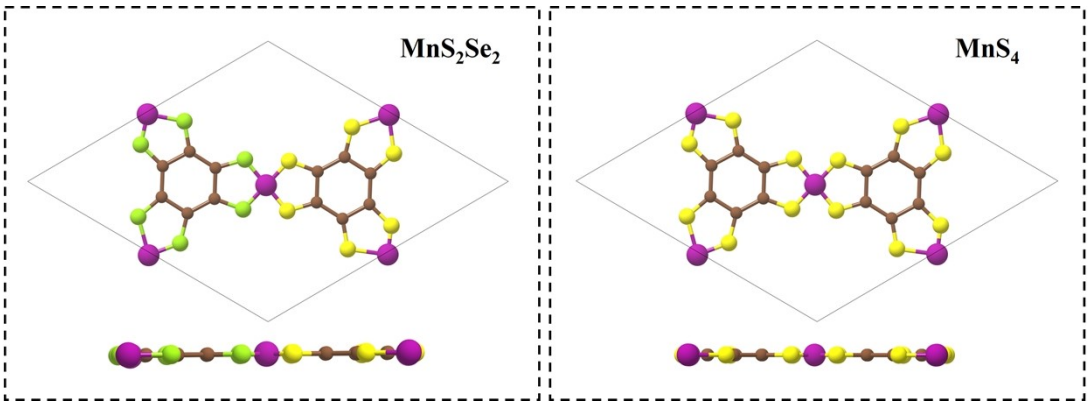

Fig. S1 Front and side views of ten different catalysts.

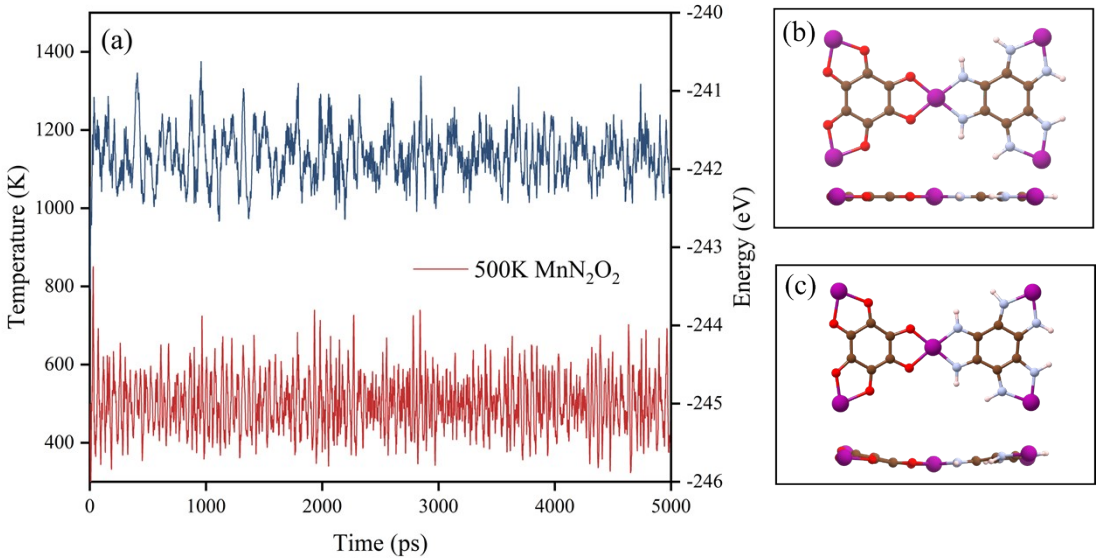

Fig. S2 (a) AIMD trajectory distribution of MnN_2O_2. (b–c) Top and side views of the structure before and after the AIMD simulation, respectively.

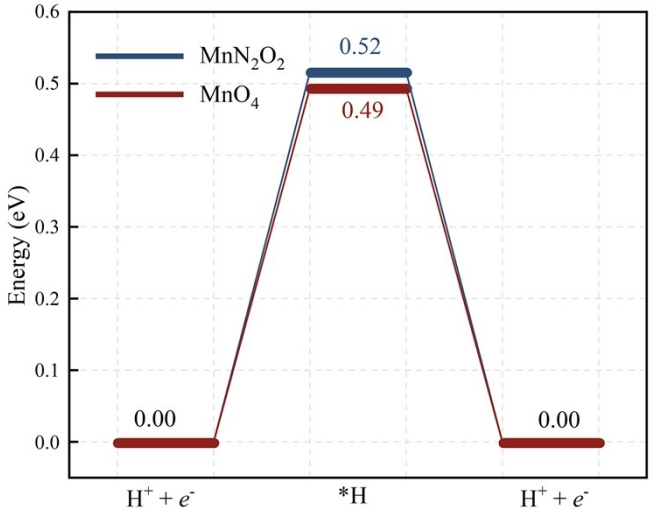

Fig. S3 Free energy step diagram for the HER competitive reaction.

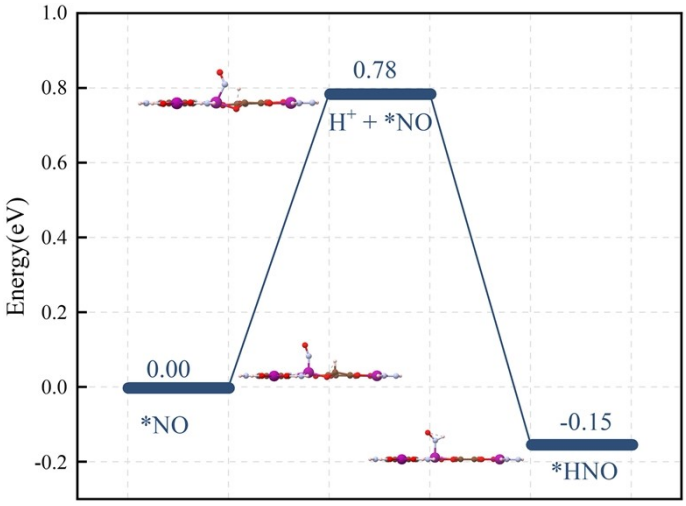

Fig. S4 Kinetic energy barrier diagram for the first-step protonation process of NO in the MnN_2O_2 system.

Table S1 MnN_2O_2, MnN_4, MnN_2S_2, MnO_4, MnS_4, MnO_2S_2, MnN_2Se_2, MnS_2Se_2, MnO_2Se_2 electronic properties of the structures, thermodynamic stability, and electrochemical descriptors.

Structure	Q_{Mn} (e)	$Q_{sum(A/B)}$ (e)	M_{Mn} (μ_B)	E_f (eV)	U_{diss} (V)
MnN_4	1.41	-4.95	3.08	-3.72	0.67
MnN_2O_2	1.50	-4.55	3.25	-3.79	0.70
MnN_2S_2	1.27	-2.97	3.28	-3.79	0.71
MnN_2Se_2	1.18	-2.76	3.35	-3.06	0.34
MnO_4	1.58	-4.09	3.33	-3.44	0.53
MnO_2S_2	1.34	-2.45	3.38	-3.46	0.54
MnO_2Se_2	1.25	-2.21	3.46	-2.77	0.19
MnS_4	1.11	-0.72	3.35	-3.50	0.56
MnS_2Se_2	1.02	-0.51	3.39	-2.81	0.22
$MnSe_4$	0.95	-0.32	3.44	-2.12	-0.13