Supplementary Material

Non-Metal Single Atoms Anchored on Defective MoS_2: A Novel Electrocatalyst for NO Reduction to NH_3

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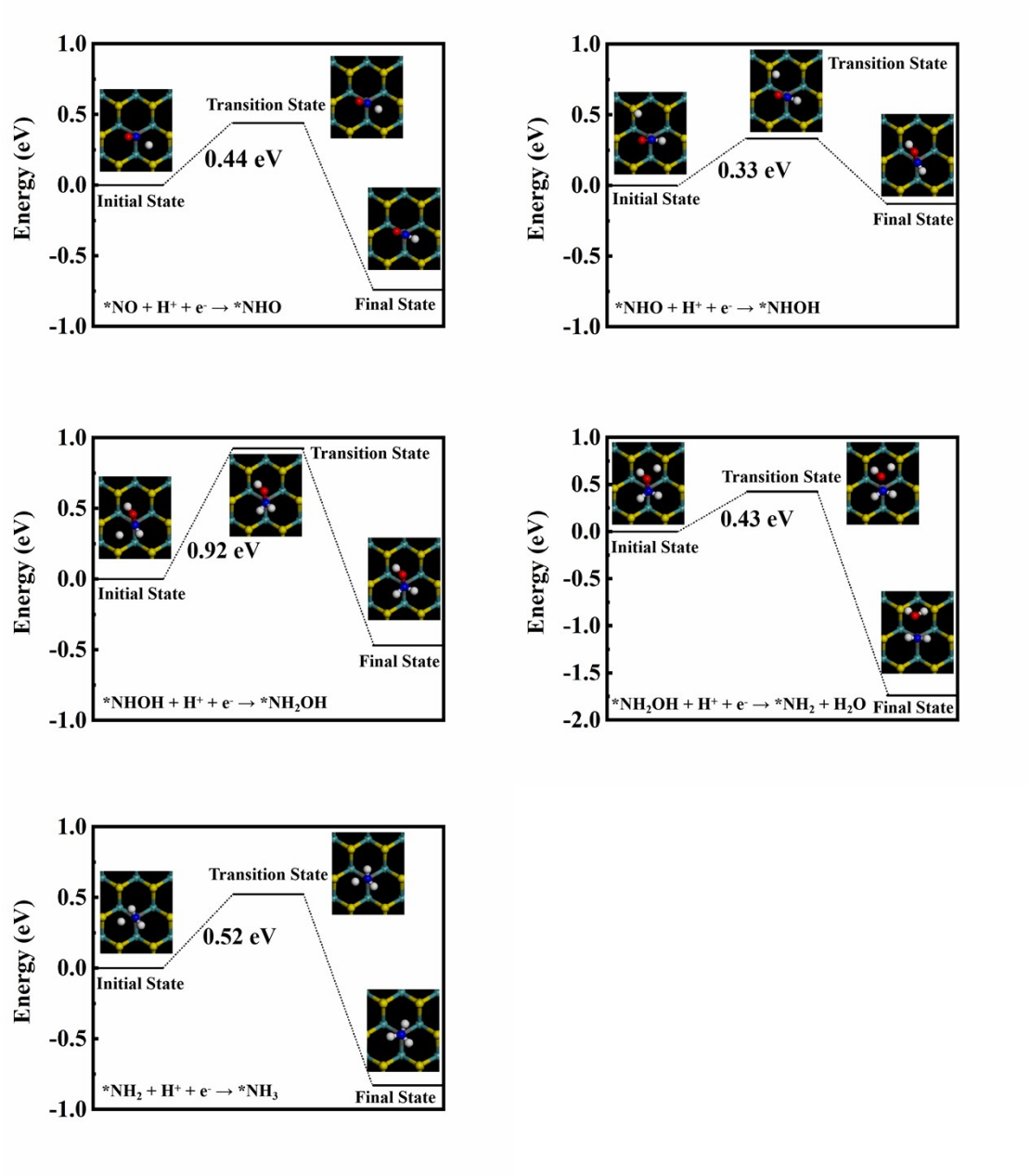

Figure S1 Energy Barriers (E_B) of each elementary reaction steps for C@MoS_2.

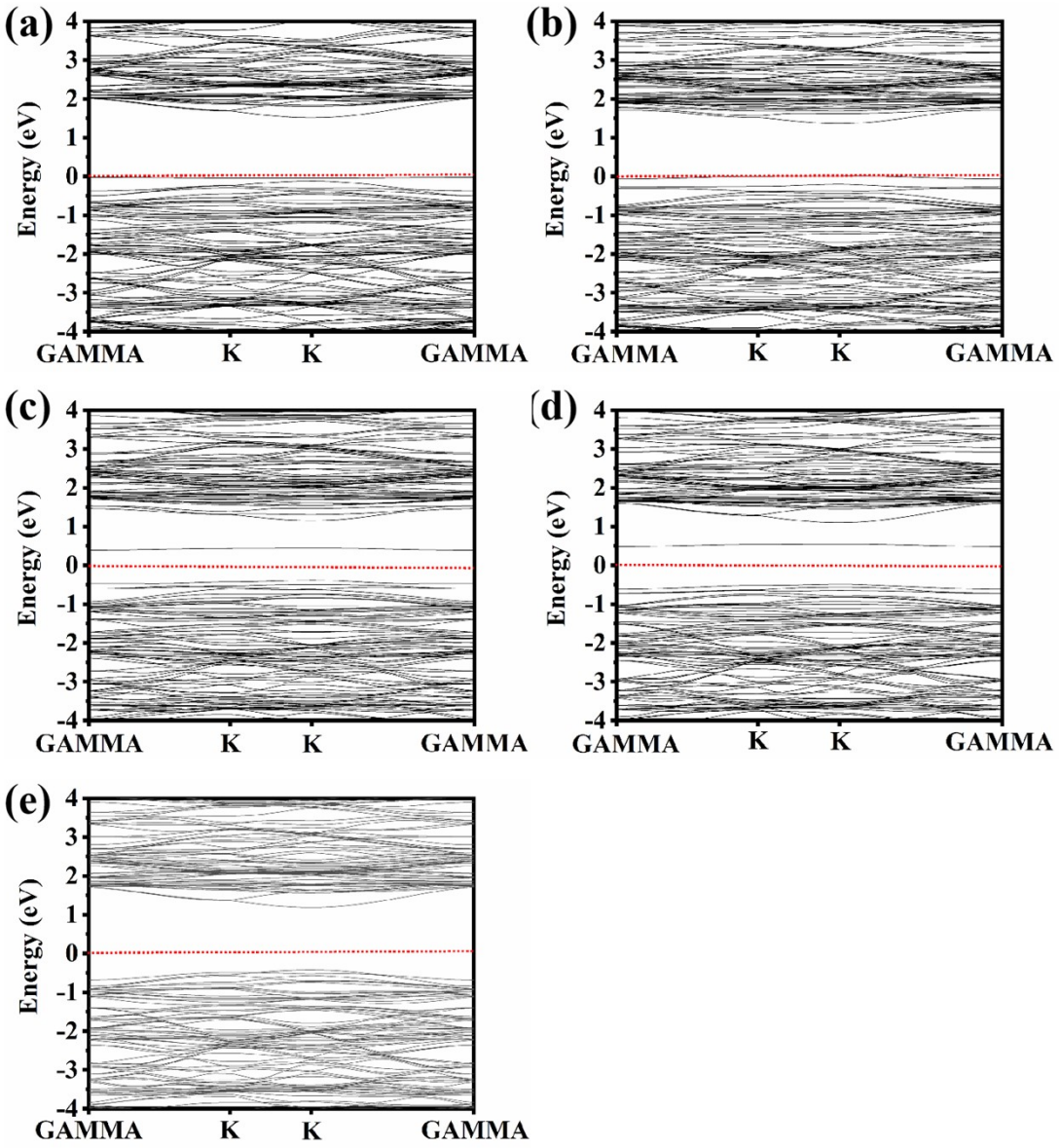

Figure S2 Band structures of (a) P@MoS_2, (b) B@MoS_2, (c) Si@MoS_2, (d) C@MoS_2, and (e) N@MoS_2 catalysts. (The red dotted line represents the Fermi level.)

Table S1 At low NO coverage, free energy changes (ΔG) of all eNORR elementary steps for NM@MoS_2 (NM=B, C, N, P, and Si).

ΔG (eV)	**B**	**C**	**N**	**P**	**Si**
*+NO→*NO (N-end)	-3.00	-1.55	-0.97	-0.93	-0.65
*NO+H^++e^-→*NOH	0.75	-0.61	0.03	-0.32	-0.17
*NO+H^++e^-→*NHO	0.62	-0.74	-0.02	-0.51	-0.63
*NOH+H^++e^-→*N+H_2O	-1.25	-0.99	-0.73	-0.18	0.15
*NOH+H^++e^-→*NHOH	-0.98	-0.26	-0.52	-1.00	-1.11
*NHO+H^++e^-→*NHOH	-0.85	-0.13	-0.47	-0.81	-0.65
NHO+H^++e^-→NH_2O	0.67	1.14	-0.14	-0.09	-1.01
*N+H^++e^-→*NH	-0.67	-0.15	-0.59	-1.62	-1.94
*NHOH+H^++e^-→*NH+H_2O	-0.94	-0.88	-0.79	-0.80	-0.67
NHOH+H^++e^-→NH_2OH	0.02	-0.47	0.30	0.80	-0.70
NH_2OH+H^++e^-→NH_2+H_2O	-2.26	-1.74	-2.44	-3.36	-1.87
NH+H^++e^-→NH_2	-1.29	-1.33	-1.34	-1.75	-1.90
NH_2O+H^++e^-→NH_2OH	-1.50	-1.74	-0.02	0.08	-0.33
NH_2+H^++e^-→NH_3	-0.41	-0.83	0.36	0.70	-1.18
NH_3→+NH_3	2.25	1.86	-0.36	0.51	2.07

Table S2 At high NO coverage, free energy changes (ΔG) of all eNORR elementary steps for NM@MoS_2 (NM=B, C, N, P, and Si).

ΔG (eV)	**B**	**C**	**P**	**Si**	**N**
+2NO→N_2O_2(2N-end)	-1.28	/	/	-0.83	/
*N_2O_2+H^++e^-→*NONOH	-1.53	//	//	-1.16	//
NONOH+H^++e^-→N_2O	-1.72	//	//	-1.66	//
N_2O+H^++e^-→N_2OH	-0.73	//	//	-0.27	//
N_2OH+H^++e^-→N_2	-1.88	//	//	-2.12	//
+2NO→N_2O_2(2O-end)	-3.27	-0.24	-1.43	-2.56	/
*N_2O_2+H^++e^-→*O	-1.30	-3.13	-1.93	-0.53	//
*O+H^++e^-→*OH	-0.36	-0.29	-1.10	-1.25	//
OH+H^++e^-→H_2O	1.62	0.35	1.16	1.04	//

The notation "/" indicates that the configuration is unstable and therefore not considered, whereas "//" indicates that subsequent hydrogenation steps are not taken into account.