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supplementary information

Electrochemical NO-to-NH_3 Conversion on TM@NiN_2 Single-Atom Catalysts: A DFT and Machine Learning Investigation

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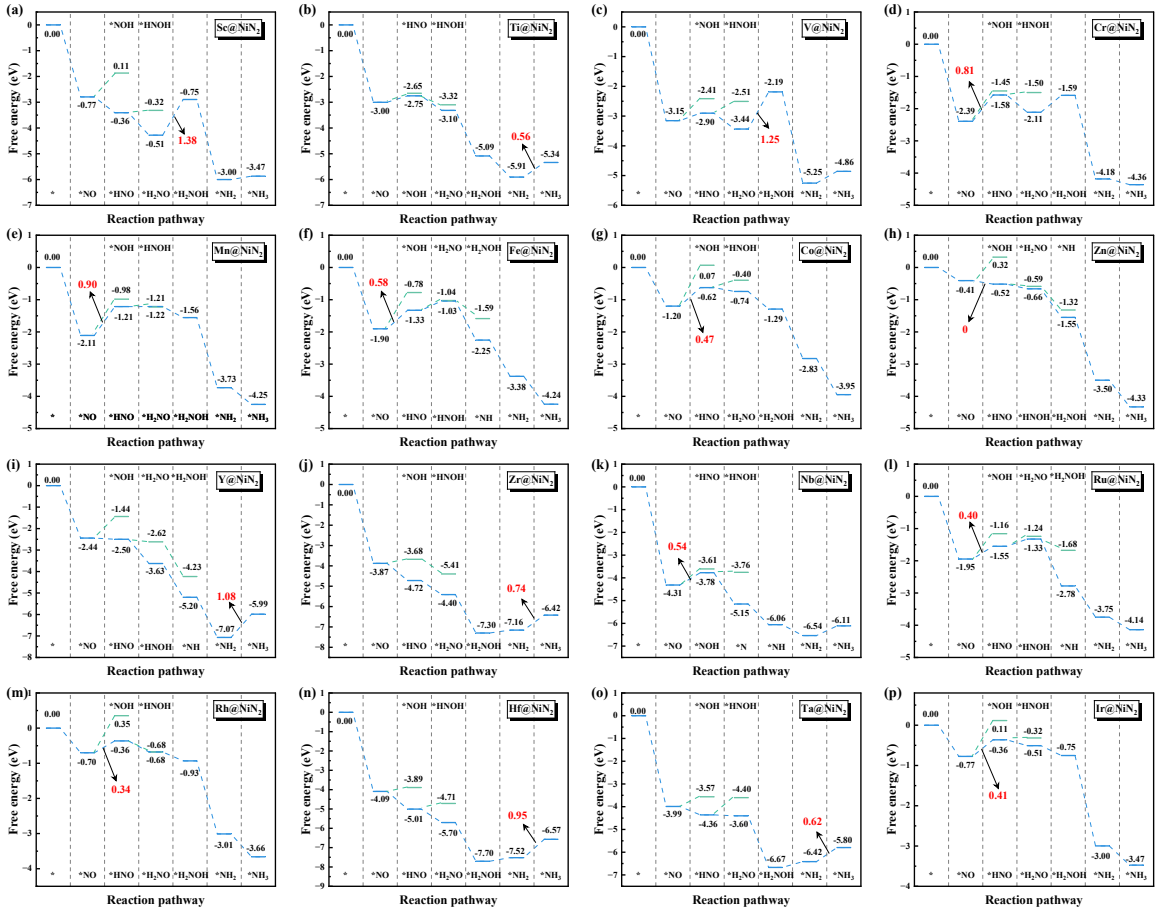

Fig. S1 (a-p) Calculated free energy diagrams for NORR by TM@NiN_2. Red numbers represent the ΔG_{max}.

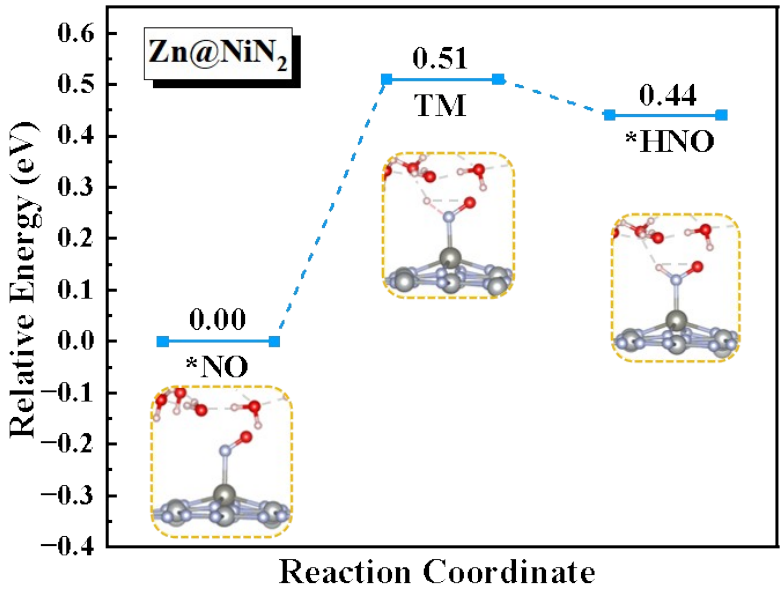

Fig. S2 Transition state search for the *NO to *HNO step under the explicit solution model.

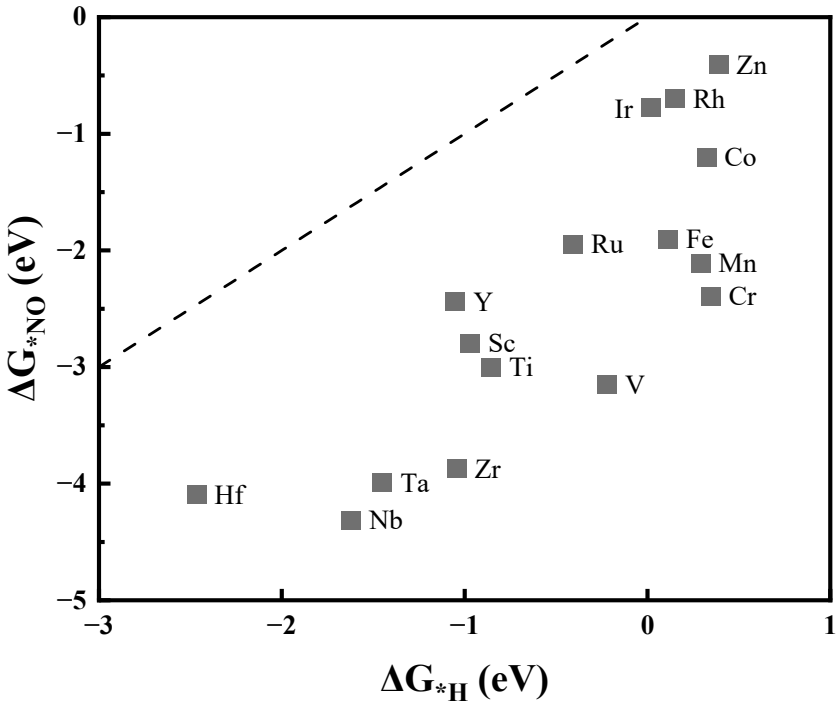

Fig. S3 Adsorption free energies of NO and H atom.

Fig. S4 Correlation heatmap of ten descriptors.

Table S1 The average distance between TM atoms and surrounding N atoms (d_N, Å).

TM	d_{TM-N1}	d_{TM-N2}	d_{TM-N3}	d_{TM-N4}	d_N
Sc	2.05	2.05	2.05	2.05	2.05
Ti	1.99	1.99	1.99	1.99	1.99
V	1.97	1.97	1.97	1.97	1.97
Cr	1.96	1.96	1.96	1.96	1.96
Mn	1.91	1.91	1.91	1.91	1.91
Fe	1.87	1.87	1.87	1.87	1.87
Co	1.85	1.85	1.85	1.85	1.85
Ni	1.88	1.88	1.88	1.88	1.88
Cu	1.93	1.93	1.93	1.93	1.93
Zn	1.98	1.98	1.98	1.98	1.98
Y	2.14	2.14	2.14	2.14	2.14
Zr	2.07	2.07	2.07	2.07	2.07
Nb	2.03	2.03	2.03	2.03	2.03
Ru	1.95	1.95	1.95	1.95	1.95
Rh	1.94	1.94	1.94	1.94	1.94
Pd	1.97	1.97	1.97	1.97	1.97
Hf	2.07	2.07	2.07	2.07	2.07
Ta	2.10	1.96	1.91	2.15	2.03

Ir	1.94	1.94	1.94	1.94	1.94
Pt	1.97	1.97	1.97	1.97	1.97
Au	2.01	2.01	2.01	2.01	2.01

Table S2 The electronegativity (χ_m), first ionization energy (E_i, eV), atomic radius (r_d, Å), magnetic moment (μ_{TM}, μ_B), electron affinity (E_a, eV), d-band center (ε_d, eV), number of d-electrons (N_d), atomic mass (m), as well as the electron transfer between TM atoms and the substrate (Q_s, e^-).

TM	N_d	r_{TM}	μ_{TM}	χ_m	E_i	E_a	m	Q_s	ε_d
Sc	1.00	1.62	0.00	1.36	6.56	0.19	44.96	1.85	1.21
Ti	2.00	1.46	2.30	1.54	6.83	0.08	47.88	1.79	0.54
V	3.00	1.35	3.89	1.63	6.74	0.53	50.94	1.43	0.83
Cr	5.00	1.28	4.45	1.66	6.76	0.67	52.00	1.31	0.15
Mn	5.00	1.26	2.34	1.55	7.43	-0.50	54.94	1.29	-0.55
Fe	6.00	1.27	1.05	1.83	7.90	0.15	55.85	1.02	-0.70
Co	7.00	1.25	0.08	1.88	7.86	0.67	58.93	0.84	-0.81
Zn	10.00	1.34	0.00	1.65	9.39	-0.54	65.41	1.10	-6.68
Y	1.00	1.80	0.00	1.22	6.22	0.31	88.91	2.04	1.10
Zr	2.00	1.60	1.64	1.33	6.95	0.43	91.22	2.10	0.45
Nb	4.00	1.47	2.59	1.60	6.77	0.89	92.91	1.74	0.09
Ru	7.00	1.34	1.00	2.20	7.36	1.06	101.10	0.96	-1.06
Rh	8.00	1.35	0.00	2.28	7.46	1.14	102.90	0.71	-1.52
Hf	2.00	1.58	1.77	1.30	7.00	0.01	178.50	1.88	0.81
Ta	3.00	1.47	2.55	1.50	7.88	0.32	180.90	1.78	0.21
Ir	7.00	1.36	0.00	2.20	9.00	1.57	192.20	0.73	-1.85

Table S3 Fitting parameter for the quadratic function of the potential-dependent energy of the Zn@NiN_2 system, of the form $E = I + b_1U + b_2U^2$.

Species	I	b_1	b_2	R^2	PZC
slab	-385.47	-1.37	-1.07	0.9957	-0.64
*NO	-398.24	-0.99	-1.16	0.9971	-0.42
*HNO	-402.29	-0.95	-1.15	0.9977	-0.41
*HNNH	-406.38	-1.36	-1.31	0.9986	-0.52
*H_2NOH	-411.34	-1.47	-1.01	0.9958	-0.73
*NH_2	-400.94	-0.75	-0.98	0.9927	-0.39
*NH_3	-406.55	-1.56	-1.01	0.9952	-0.77
*H	-388.32	-0.63	-0.92	0.9894	-0.34