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Supporting Information

For

A theoretical investigation on the OER and ORR activity of graphene-based TM-N_3 and TM-N_2X (X=B, C, O, P) single atom catalysts by density functional theory calculations

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Table S1. The formation energy (E_f) of transition metals. The theoretical overpotential (η), Gibbs free energy change of the oxygenated intermediates (ΔG_{*OOH}, ΔG_{*O}, ΔG_{*OH}).

	E_b(eV)	η_{OER}(V)	η_{ORR}(V)	G_{*OH}(eV)	G_{*O}(eV)	G_{*OOH}(eV)	$*O_2$(eV)
TiN_2B	-2.37	2.40	2.01	-0.78	0.20	3.63	1.87
VN_2B	-2.56	2.48	2.16	-0.93	0.48	3.71	1.66
CrN_2B	-2.33	1.77	1.69	-0.46	0.78	3.00	1.60
MnN_2B	-0.96	2.75	1.19	0.41	0.49	3.98	0.04
FeN_2B	-2.36	2.18	1.13	0.10	0.30	3.41	1.11
CoN_2B	-2.33	1.57	1.22	0.01	0.96	2.80	1.15
NiN_2B	-1.67	0.93	0.69	0.54	1.59	2.16	0.63
CuN_2B	-1.36	0.50	0.87	0.90	1.93	1.73	0.36
TiN_2C	-4.10	2.46	2.31	-1.08	0.37	3.69	1.94
VN_2C	-4.42	2.35	2.21	-0.98	0.47	3.58	1.85
CrN_2C	-4.00	2.16	1.72	-0.49	0.21	3.39	1.81
MnN_2C	-3.11	2.20	1.77	-0.54	0.35	3.43	1.68
FeN_2C	-3.57	2.14	1.42	-0.19	0.44	3.37	1.30
CoN_2C	-2.41	3.19	1.66	-0.43	4.42	-0.37	1.30
NiN_2C	-1.67	1.10	0.65	0.59	1.42	2.33	0.58
CuN_2C	0.38	2.34	2.59	0.91	1.80	3.57	-1.36

TiN_3	-3.83	4.73	2.81	-1.58	0.52	0.02	5.96
VN_3	-6.91	3.44	2.04	1.32	-0.81	4.67	-0.26
CrN_3	-6.17	0.26	0.67	1.49	0.56	1.48	1.39
MnN_3	-5.68	1.26	1.04	1.14	1.10	2.49	0.19
FeN_3	-4.02	1.22	2.12	-0.89	1.20	2.45	2.16
CoN_3	-3.67	1.12	0.77	0.46	1.20	2.35	0.91
NiN_3	-1.35	0.89	1.18	0.05	1.51	2.12	1.24
CuN_3	-0.53	0.31	0.44	0.79	1.53	1.54	1.06
TiN_2O	0.54	2.78	2.60	-1.37	0.36	4.01	1.92
VN_2O	0.18	2.47	2.24	-1.01	0.29	3.70	1.93
CrN_2O	0.43	1.97	1.89	-0.66	0.75	3.20	1.63
MnN_2O	2.37	2.11	2.19	-0.96	0.62	3.34	1.92
FeN_2O	1.27	2.55	3.18	-1.95	1.49	3.78	1.60
CoN_2O	1.55	0.94	1.62	-0.39	1.53	2.17	1.62
NiN_2O	2.97	0.81	1.11	0.12	1.28	2.04	1.48
CuN_2O	2.28	0.77	1.04	0.19	2.02	2.00	0.71
TiN_2P	2	2.12	2.30	-1.07	0.53	3.35	2.11
VN_2P	2.05	1.67	2.03	-0.80	0.94	2.90	1.88
CrN_2P	2.04	1.99	0.97	0.26	0.73	3.22	0.71
MnN_2P	2.64	2.30	2.70	-1.47	1.46	3.53	1.40
FeN_2P	2.09	1.31	0.67	0.56	1.04	2.54	0.78
CoN_2P	0.98	1.05	0.47	1.09	0.76	2.28	0.79
NiN_2P	0.29	0.66	0.63	0.60	1.78	1.89	0.65
CuN_2P	0.45	0.72	0.87	0.72	1.89	1.95	0.36

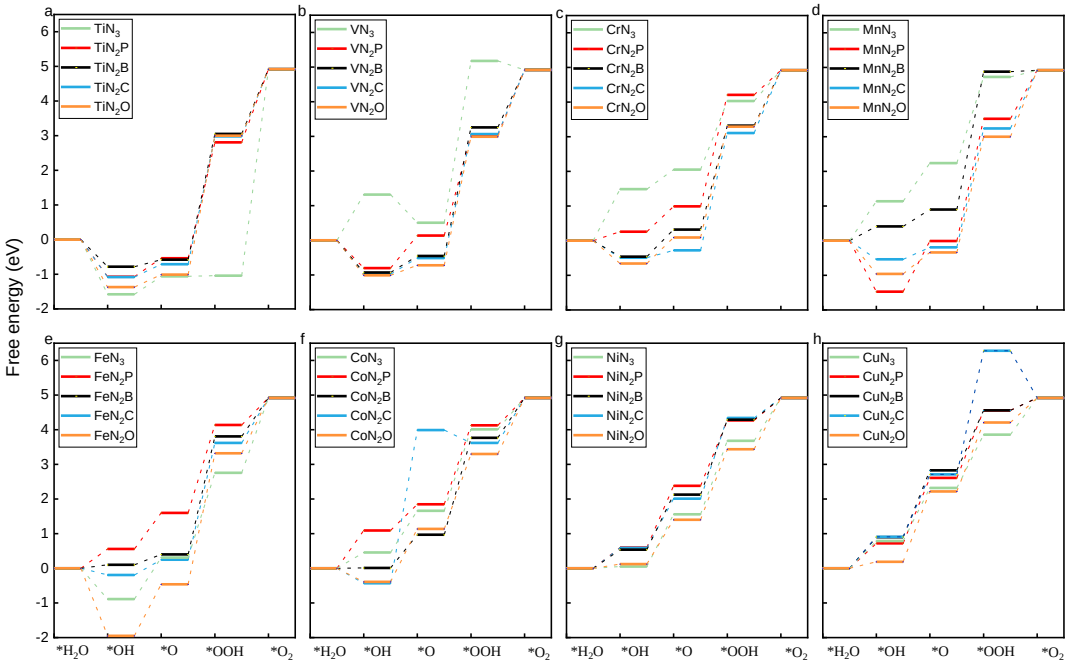

Figure S1. Calculated the free energy profile of TMN_2X.