

Supporting Information

Tailoring OER/ORR Activity in TM_1N_4 Catalysts through First-/Second-Shell

Nitrogen Doping: A Density Functional Theory Investigation

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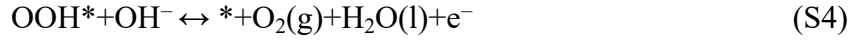
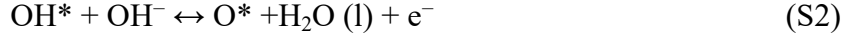
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Simulation Details

The electrochemical model of OER/ORR in alkaline media could be divided into the four one-electron reactions:



where the * denoted the active site. The adsorption energies of intermediates (OH, O and OOH groups) on substrates were calculated by following:

$$\Delta E_{*O} = E(\text{sub/O}) - E(\text{sub}) - [E(\text{H}_2\text{O}) - E(\text{H}_2)] \quad (\text{S5})$$

$$\Delta E_{*OH} = E(\text{sub/OH}) - E(\text{sub}) - [E(\text{H}_2\text{O}) - E(\text{H}_2)/2] \quad (\text{S6})$$

$$\Delta E_{*OOH} = E(\text{sub/OOH}) - E(\text{sub}) - [2 \times E(\text{H}_2\text{O}) - 3 \times E(\text{H}_2)/2] \quad (\text{S7})$$

where $E(\text{sub/H}_2\text{O})$, $E(\text{sub/OH})$, $E(\text{sub/O})$ and $E(\text{sub/OOH})$ denoted the total energies of H_2O , OH, O and OOH groups on substrates. $E(\text{sub})$, $E(\text{H}_2\text{O})$ and $E(\text{H}_2)$ were the energies of bare substrate, water, and hydrogen gas, respectively.

The Gibbs free energy changes of steps S1-S4 could be estimated by:

$$\Delta G_1 = \Delta G_{\text{OH}^*} \quad (\text{S8})$$

$$\Delta G_2 = \Delta G_{\text{O}^*} - \Delta G_{\text{OH}^*} \quad (\text{S9})$$

$$\Delta G_3 = \Delta G_{\text{OOH}^*} - \Delta G_{\text{O}^*} \quad (\text{S10})$$

$$\Delta G_4 = 4.92 \text{ eV} - \Delta G_{\text{OOH}^*} \quad (\text{S11})$$

where the sum of ΔG_{1-4} was fixed to the negative of experimental Gibbs free energy of formation of two water molecules ($-2 \Delta_{\text{H}_2\text{O}}^{\text{exp}} = 4.92 \text{ eV}$). The Gibbs free energy of ($\text{H}^+ + \text{e}^-$) in solution was estimated as the half energy of H_2 molecule at standard condition.

The overpotential of OER was determined by following equations:

$$\eta^{\text{OER}} = U_{\text{OER}} - 1.23 \quad (\text{S12})$$

$$U_{\text{OER}} = \text{Max}(\Delta G_1, \Delta G_2, \Delta G_3, \Delta G_4)/e \quad (\text{S13})$$

The overpotential of ORR was expressed as:

$$\eta^{\text{ORR}} = 1.23 - U_{\text{ORR}} \quad (\text{S14})$$

$$U_{\text{ORR}} = \text{Min}(\Delta G_1, \Delta G_2, \Delta G_3, G_4)/e \quad (\text{S15})$$

The proportional relationships between the ΔG_{O^*} , ΔG_{OH^*} and ΔG_{OOH^*} values:

$$\Delta G_{\text{OH}^*} = 0.611 \times \Delta G_{\text{O}^*} - 0.557 \quad (\text{S16})$$

$$\Delta G_{\text{OOH}^*} = 0.510 \times \Delta G_{\text{O}^*} + 2.431 \quad (\text{S17})$$

The proportional relationships between the ΔG and D_d values:

$$\Delta G_{\text{OH}^*} = 0.088 \times D_d - 1.124 \quad (\text{S18})$$

$$\Delta G_{\text{O}^*} = 0.141 \times D_d - 0.849 \quad (\text{S19})$$

$$\Delta G_{\text{OOH}^*} = 0.079 \times D_d + 1.806 \quad (\text{S20})$$

Table S1. The formation energy of all systems.

Coordination Environment	Dopant Position	E_{system} (eV)	E_{C} (eV)	E_{N} (eV)	E_{TM} (eV)	ΔE_{form} (eV)
Fe ₁ -pyridine N ₄	Pristine	-13528.163	-145.717	-261.366	-2856.365	-9.012
	N1 site	-13643.767				-8.967
	N2 site	-13643.775				-8.975
	N3 site	-13643.779				-8.979
Co ₁ -pyridine N ₄	Pristine	-11187.764			-515.957	-9.021
	N1 site	-11303.357				-8.965
	N2 site	-11303.366				-8.974
	N3 site	-11303.381				-8.989
Ni ₁ -pyridine N ₄	Pristine	-14566.938			-3895.158	-8.994
	N1 site	-14682.467				-8.874
	N2 site	-14682.585				-8.992
	N3 site	-14682.592				-8.999
Fe ₁ -pyrrolee N ₄	Pristine	-12653.816			-2856.365	-8.967
	N1 site	-12769.412				-8.914
	N2 site	-12769.419				-8.921
	N3 site	-12769.443				-8.945
Co ₁ -pyrrolee N ₄	Pristine	-10313.395	-515.957	-8.954		
	N1 site	-10428.994		-8.904		
	N2 site	-10429.007		-8.917		
	N3 site	-10429.015		-8.925		
Ni ₁ -pyrrolee N ₄	Pristine	-13692.476	-3895.158	-8.834		
	N1 site	-13808.071		-8.780		
	N2 site	-13808.085		-8.794		
	N3 site	-13808.093		-8.802		

Table S2. The lengths of $\text{TM}_1\text{-N}$ bonds ($d_{\text{TM}_1\text{-N}}$), the estimated dynamic volume of d electron (V_d) and d electron density (D_d) of each TM_1 ion.

Coordination Environment	Dopant	$d_{\text{TM}_1\text{-N}}$ (Å)				V_d (Å ³)	D_d (e/Å ³)
	Position	Bond 1	Bond 2	Bond 3	Bond 4		
Fe ₁ -pyridine N ₄	Pristine	1.891	1.891	1.891	1.891	0.918	26.144
	N1 site	1.871	1.899	1.892	1.877	0.909	26.402
	N2 site	1.894	1.886	1.886	1.894	0.917	26.185
	N3 site	1.908	1.901	1.887	1.888	0.925	25.936
Co ₁ -pyridine N ₄	Pristine	1.884	1.884	1.884	1.884	0.905	30.941
	N1 site	1.867	1.893	1.883	1.869	0.896	31.236
	N2 site	1.883	1.879	1.879	1.883	0.900	31.090
	N3 site	1.901	1.893	1.879	1.881	0.912	30.719
Ni ₁ -pyridine N ₄	Pristine	1.881	1.881	1.881	1.881	0.898	35.646
	N1 site	1.883	1.883	1.877	1.873	0.895	35.759
	N2 site	1.885	1.876	1.876	1.885	0.897	35.673
	N3 site	1.901	1.890	1.879	1.880	0.907	35.276
Fe ₁ -pyrrolee N ₄	Pristine	1.972	1.972	1.972	1.972	1.041	23.053
	N1 site	1.997	1.989	1.962	1.953	1.047	22.933
	N2 site	1.974	1.969	1.969	1.974	1.040	23.070
	N3 site	2.013	2.000	1.953	1.978	1.064	22.560
Co ₁ -pyrrolee N ₄	Pristine	1.989	1.989	1.989	1.989	1.065	26.295
	N1 site	2.020	2.005	1.977	1.968	1.071	26.148
	N2 site	1.991	1.987	1.987	1.991	1.065	26.295
	N3 site	2.033	2.018	1.968	1.994	1.088	25.726
Ni ₁ -pyrrolee N ₄	Pristine	1.955	1.955	1.955	1.955	1.008	31.749
	N1 site	1.983	1.967	1.948	1.939	1.015	31.536
	N2 site	1.954	1.953	1.953	1.954	1.006	31.822
	N3 site	1.985	1.982	1.942	1.962	1.028	31.129

Table S3. The integration of negative crystal orbitals Hamiltonian population (-ICOHP) values of TM₁-N bonds.

System	Bond	-ICOHP (eV)	System	Bond	-ICOHP (eV)	System	Bond	-ICOHP (eV)
Fe-pyridine		0.935	Co-pyridine		1.236	Ni-pyridine		0.964
N1 site	1	1.027	N1 site	1	1.275	N1 site	1	0.968
	2	0.908		2	1.193		2	0.914
	3	0.919		3	1.211		3	0.921
	4	0.891		4	1.198		4	0.901
N2 site	1	0.841	N2 site	1	1.139	N2 site	1	0.864
	2	0.891		2	1.191		2	0.916
	3	0.892		3	1.191		3	0.916
	4	0.841		4	1.139		4	0.864
N3 site	1	0.823	N3 site	1	1.099	N3 site	1	0.833
	2	0.907		2	1.179		2	0.913
	3	0.914		3	1.212		3	0.932
	4	0.909		4	1.192		4	0.914
Fe-pyrrolee		0.613	Co-pyrrolee		0.973	Ni-pyrrolee		0.787
N1 site	1	0.709	N1 site	1	0.998	N1 site	1	0.742
	2	0.578		2	0.976		2	0.751
	3	0.598		3	0.988		3	0.749
	4	0.522		4	0.916		4	0.705
N2 site	1	0.505	N2 site	1	0.889	N2 site	1	0.677
	2	0.561		2	0.945		2	0.725
	3	0.561		3	0.945		3	0.725
	4	0.505		4	0.889		4	0.677
N3 site	1	0.532	N3 site	1	0.903	N3 site	1	0.689
	2	0.588		2	0.967		2	0.752
	3	0.607		3	0.986		3	0.767
	4	0.578		4	0.964		4	0.753

Table S4. The free energy of each intermediate (ΔG_{OH^*} , ΔG_{O^*} or ΔG_{OOH^*}), the free energy change of each elemental step (ΔG_1 , ΔG_2 , ΔG_3 or ΔG_4) and the reaction overpotentials of OER (η^{OER}) and ORR (η^{ORR}).

Coordination Environment	Dopant Position	ΔG_{OH^*} (eV)	ΔG_{O^*} (eV)	ΔG_{OOH^*} (eV)	ΔG_1 (eV)	ΔG_2 (eV)	ΔG_3 (eV)	ΔG_4 (eV)	η^{OER} (V)	η^{ORR} (V)
Fe ₁ -pyridine N ₄	Pristine	1.021	2.517	3.867	1.021	1.496	1.350	1.053	0.266	0.209
	N1 site	1.096	2.702	3.967	1.096	1.606	1.265	0.953	0.376	0.277
	N2 site	1.034	2.636	3.881	1.034	1.602	1.245	1.039	0.372	0.196
	N3 site	1.011	2.484	3.821	1.011	1.473	1.337	1.099	0.243	0.219
Co ₁ -pyridine N ₄	Pristine	1.837	3.581	4.512	1.837	1.744	0.931	0.408	0.607	0.822
	N1 site	1.862	3.632	4.518	1.862	1.770	0.886	0.402	0.632	0.828
	N2 site	1.841	3.616	4.513	1.841	1.775	0.897	0.407	0.611	0.823
	N3 site	1.747	3.467	4.371	1.747	1.720	0.904	0.549	0.517	0.681
Ni ₁ -pyridine N ₄	Pristine	1.821	4.024	4.595	1.821	2.203	0.571	0.325	0.973	0.905
	N1 site	1.887	4.098	4.619	1.887	2.211	0.521	0.301	0.981	0.929
	N2 site	1.846	4.084	4.598	1.846	2.238	0.514	0.322	1.008	0.908
	N3 site	1.789	3.899	4.537	1.789	2.110	0.638	0.383	0.880	0.847
Fe ₁ -pyrrolee N ₄	Pristine	0.896	2.351	3.687	0.896	1.455	1.336	1.233	0.225	0.334
	N1 site	0.845	2.301	3.615	0.845	1.456	1.314	1.305	0.226	0.385
	N2 site	0.912	2.378	3.694	0.912	1.466	1.316	1.226	0.236	0.318
	N3 site	0.794	2.233	3.512	0.794	1.439	1.279	1.408	0.209	0.436
Co ₁ -pyrrolee N ₄	Pristine	1.228	3.142	3.845	1.228	1.914	0.703	1.075	0.684	0.527
	N1 site	1.213	3.041	3.816	1.213	1.828	0.775	1.104	0.598	0.455
	N2 site	1.232	3.155	3.871	1.232	1.923	0.716	1.049	0.693	0.514
	N3 site	1.199	2.891	3.743	1.199	1.692	0.852	1.177	0.462	0.378
Ni ₁ -pyrrolee N ₄	Pristine	1.772	3.698	4.181	1.772	1.926	0.483	0.739	0.696	0.747
	N1 site	1.732	3.678	4.177	1.732	1.946	0.499	0.743	0.716	0.731
	N2 site	1.798	3.802	4.218	1.798	2.004	0.416	0.702	0.774	0.814

	N3 site	1.689	3.647	4.148	1.689	1.958	0.501	0.772	0.728	0.729
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Table S5. The comparison of OER/ORR activity between our systems and other works.

Electrocatalysts	η^{OER} (V)	η^{ORR} (V)	Reference
N3-doped Fe ₁ -pyrrole N ₄	209		Our work
N2-doped Fe ₁ -pyridine N ₄		196	Our work
Co@N ₄ SAC	330	410	Ref [1]
IrN ₄ -C	300	N.A.	Ref [2]
g-C ₃ N ₄ (TM/VN-CN)	320	430	Ref [3]
TMN ₄ @G	260	240	Ref [4]
Ir/pyrrolic-N ₄ -G	320	340	Ref [5]
3FeCN/S	260	480	Ref [6]
TMN ₄ -gra	N.A.	339	Ref [7]
((TM-N _x O _{4-x})@g-C1 ₆ N ₃ -h ₃ , x = 0-4)	300	460	Ref [8]

Figure S1. The total energies of systems with the initial magnetic moments of Fe, Co and Ni atoms in (a) Fe₁-pyridine N₄, (c) Co₁-pyridine N₄, (e) Ni₁-pyridine N₄, (b) Fe₁-pyrrole N₄, (d) Co₁-pyrrole N₄, and (f) Ni₁-pyrrole N₄ systems.

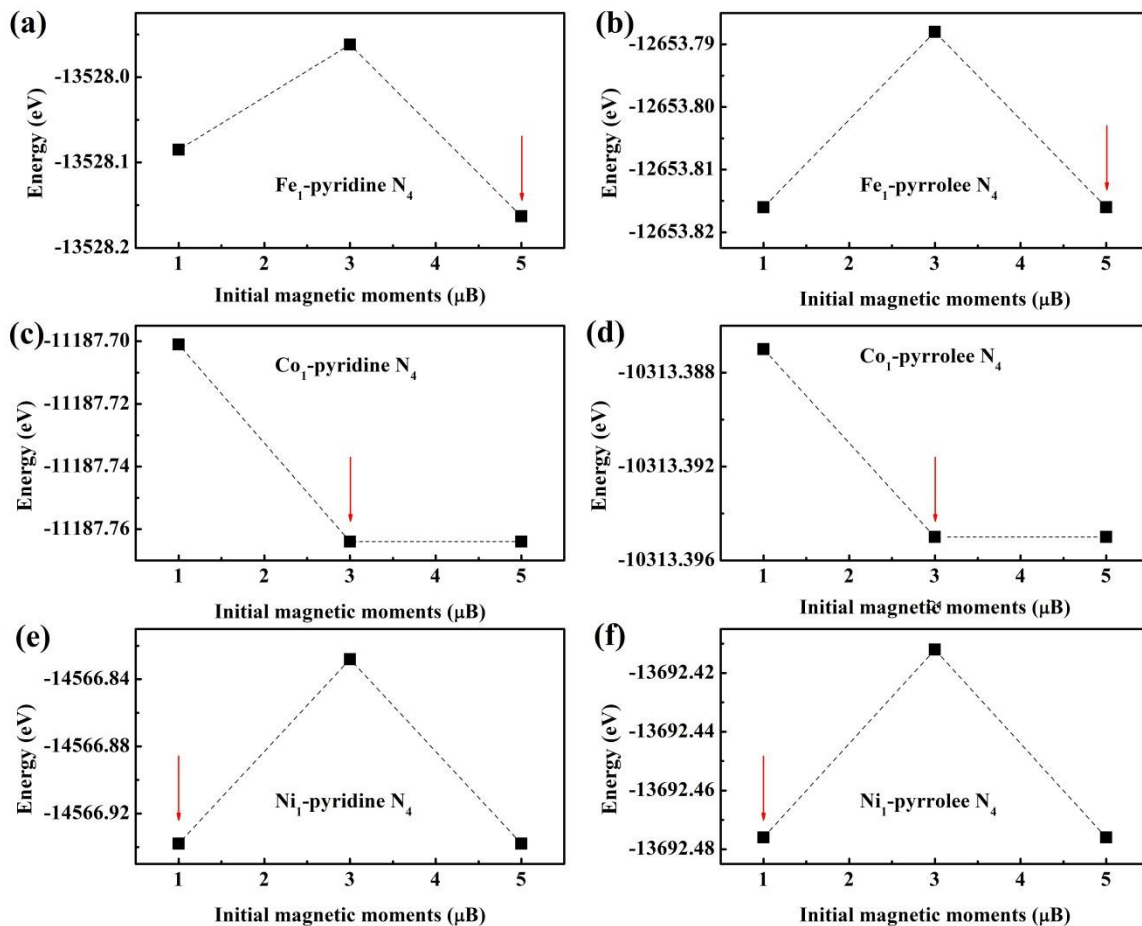


Figure S2. The changed percentages (%) of all TM_1 -N bonds. (a) bond 1, (b) bond 2, (c) bond 3 and (d) bond 4.

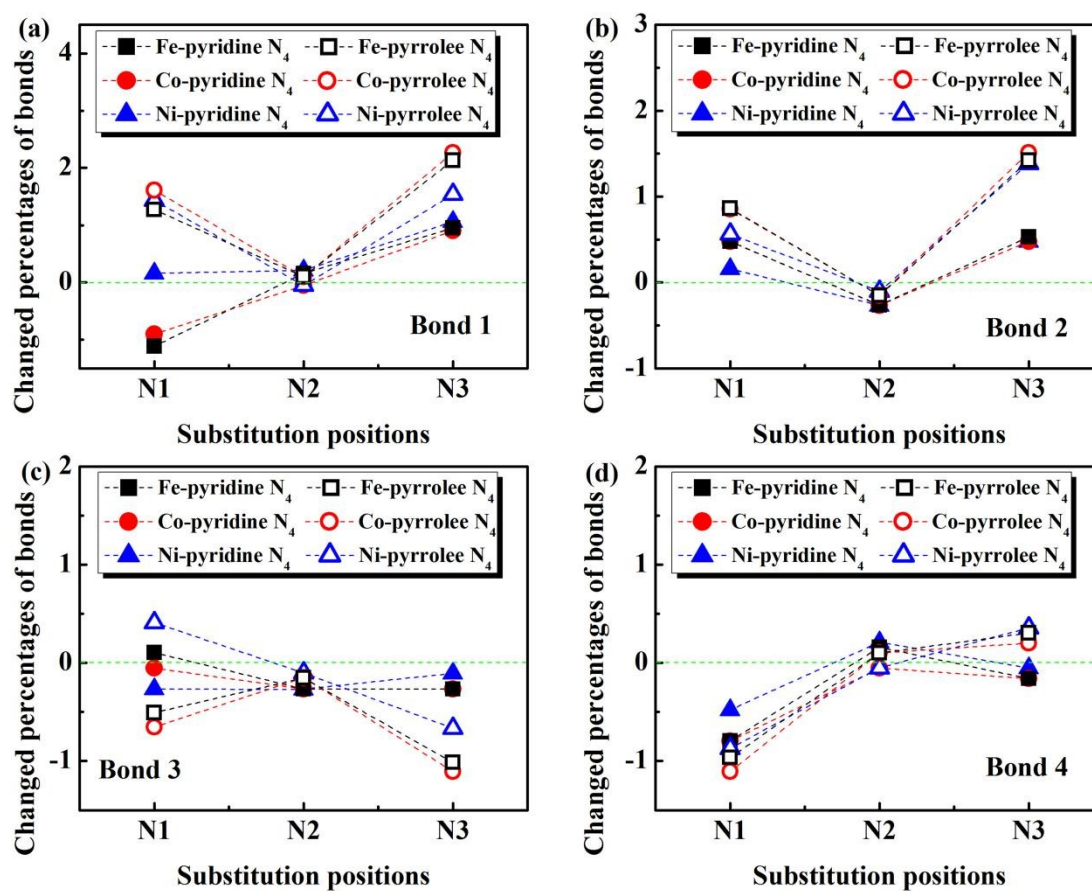


Figure S3. The negative crystal orbitals Hamiltonian population (-COHP) of Fe₁-N bonds in (a) N1 doped, (c) N2 doped and (e) N3 doped Fe₁-pyridine N₄ active centers, (b) N1 doped, (d) N2 doped and (f) N3 doped Fe₁-pyrrolee N₄ active centers, comparing for pristine active centers.

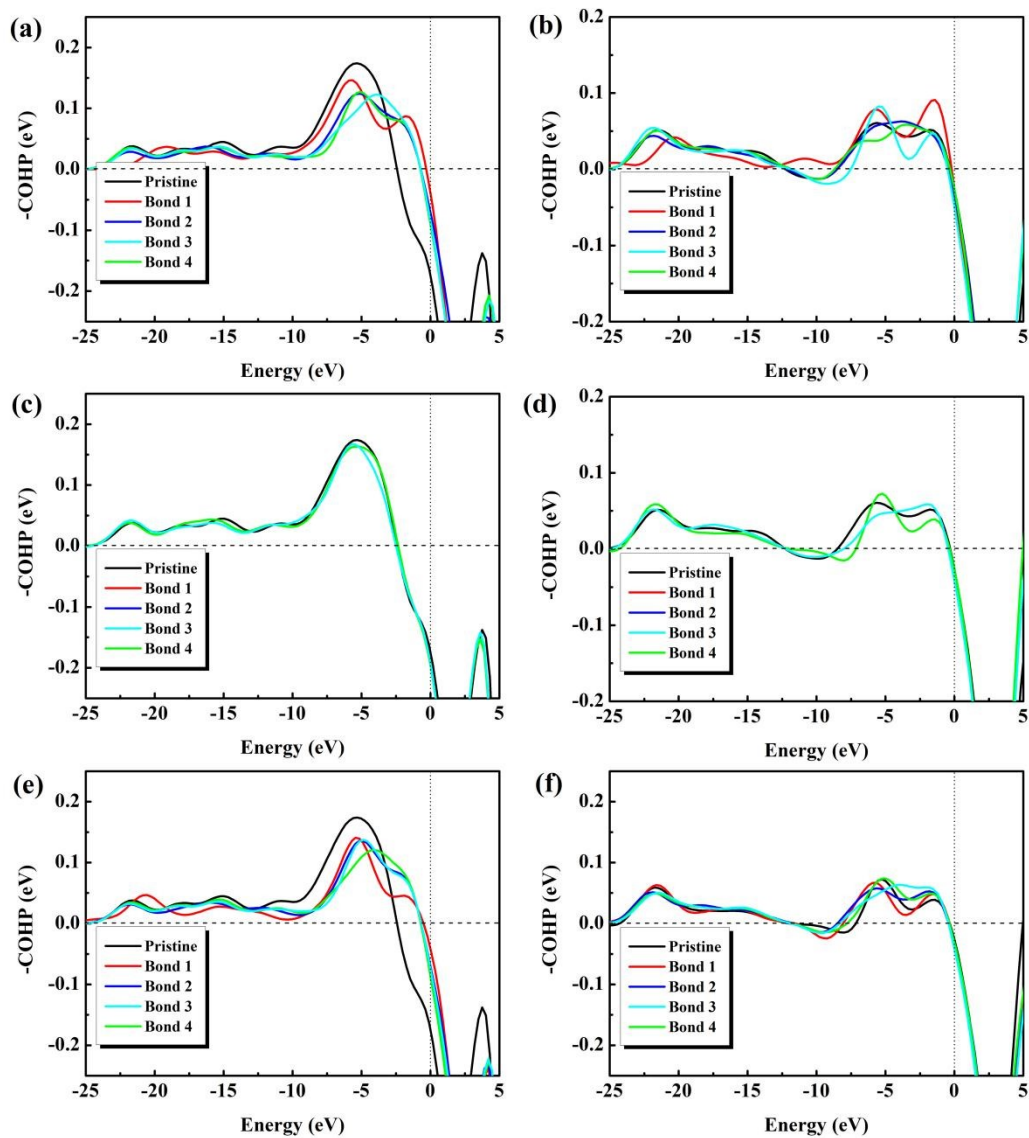


Figure S4. The negative crystal orbitals Hamiltonian population (-COHP) of Co₁-N bonds in (a) N1 doped, (c) N2 doped and (e) N3 doped Co₁-pyridine N₄ active centers, (b) N1 doped, (d) N2 doped and (f) N3 doped Co₁-pyrrolee N₄ active centers, comparing for pristine active centers.

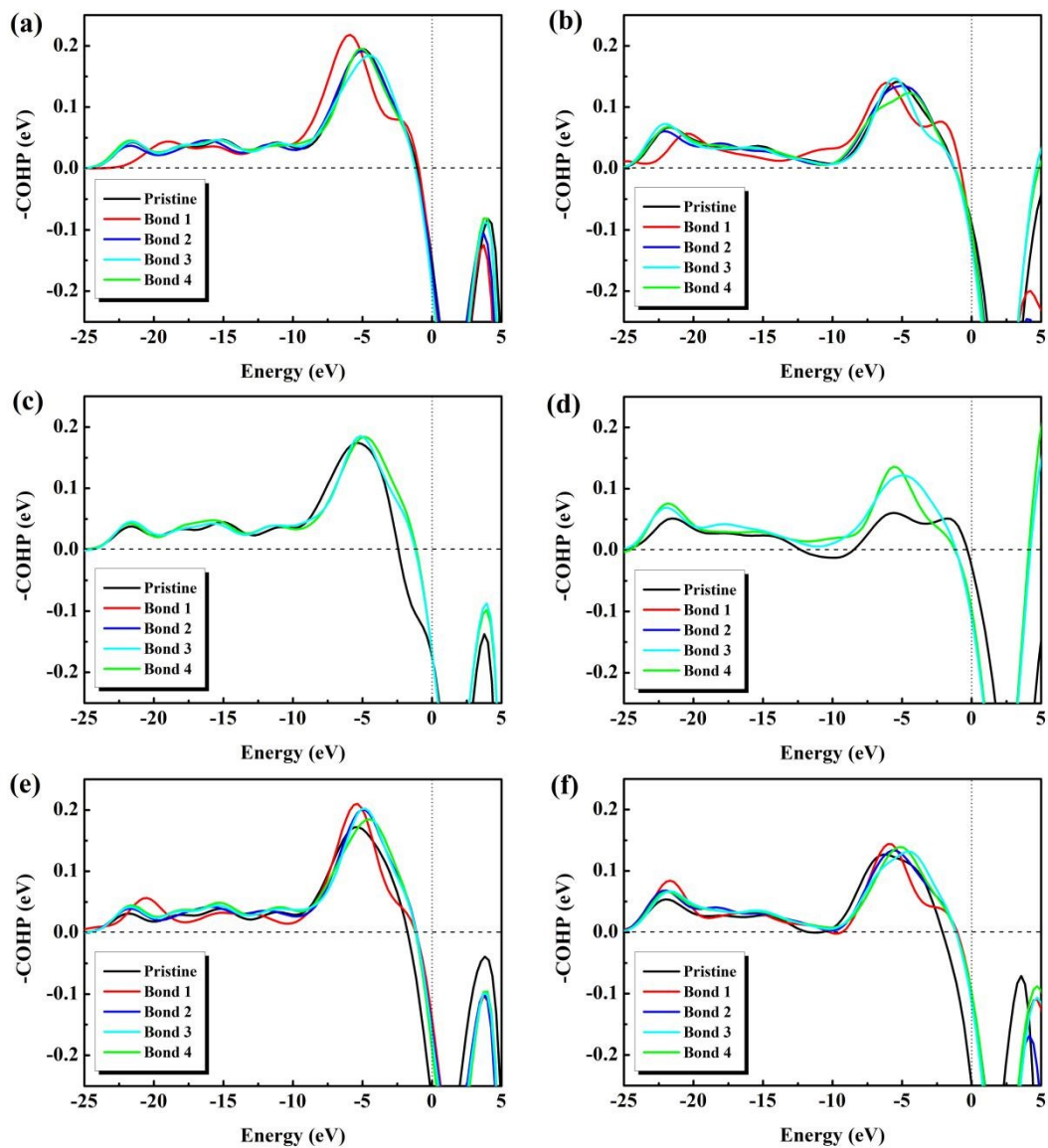


Figure S5. The negative crystal orbitals Hamiltonian population (-COHP) of Ni₁-N bonds in (a) N1 doped, (c) N2 doped and (e) N3 doped Ni₁-pyridine N₄ active centers, (b) N1 doped, (d) N2 doped and (f) N3 doped Ni₁-pyrrolee N₄ active centers, comparing for pristine active centers.

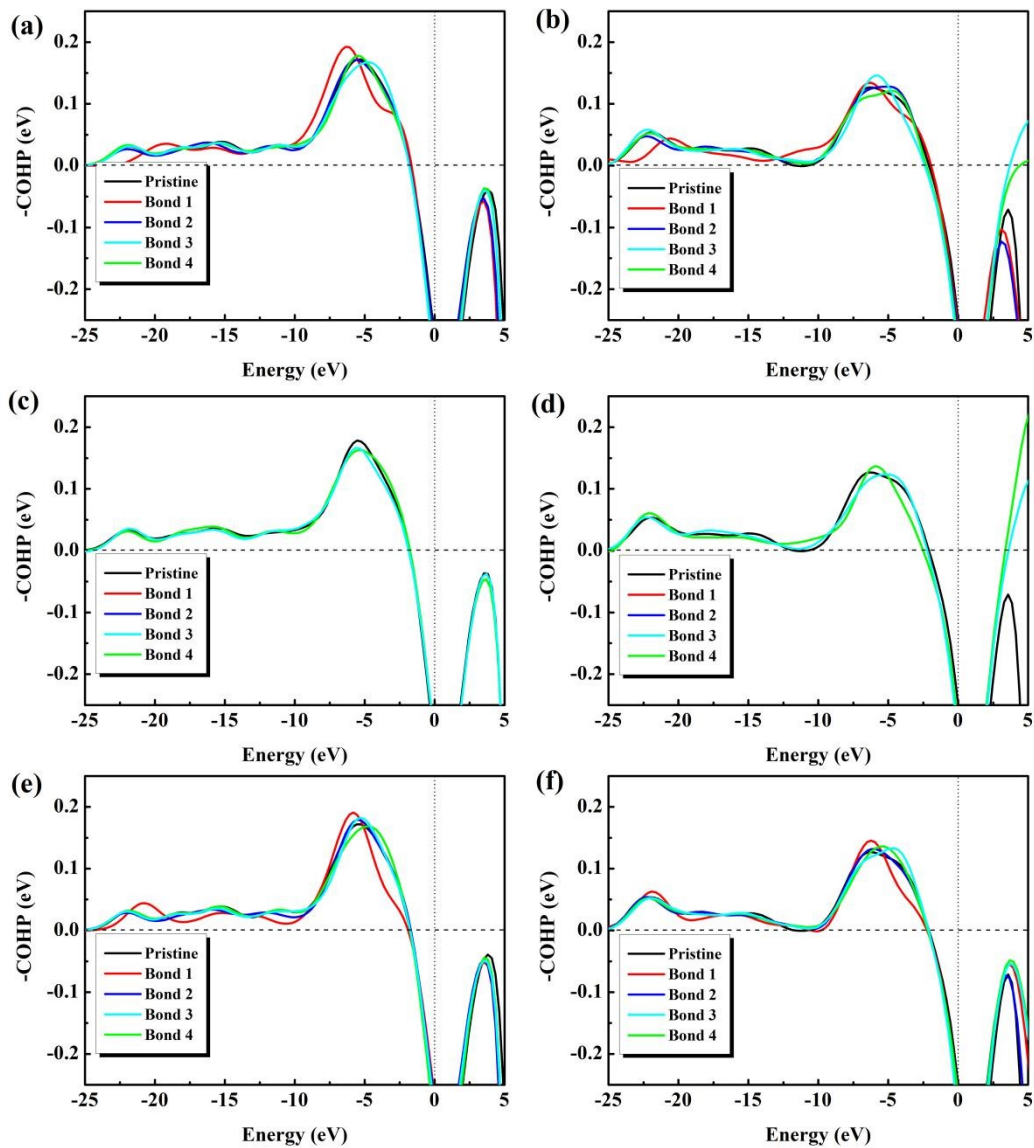


Figure S6. The atom structures of (a) $*$, (b) OH^* , (c) O^* and (d) OOH^* , $*$ denoted the active site of TM monoatom in TM_1 -pyridine N_4 systems, where the white, red, gray, blue and green balls denoted the H, O, C, N and TM atoms.

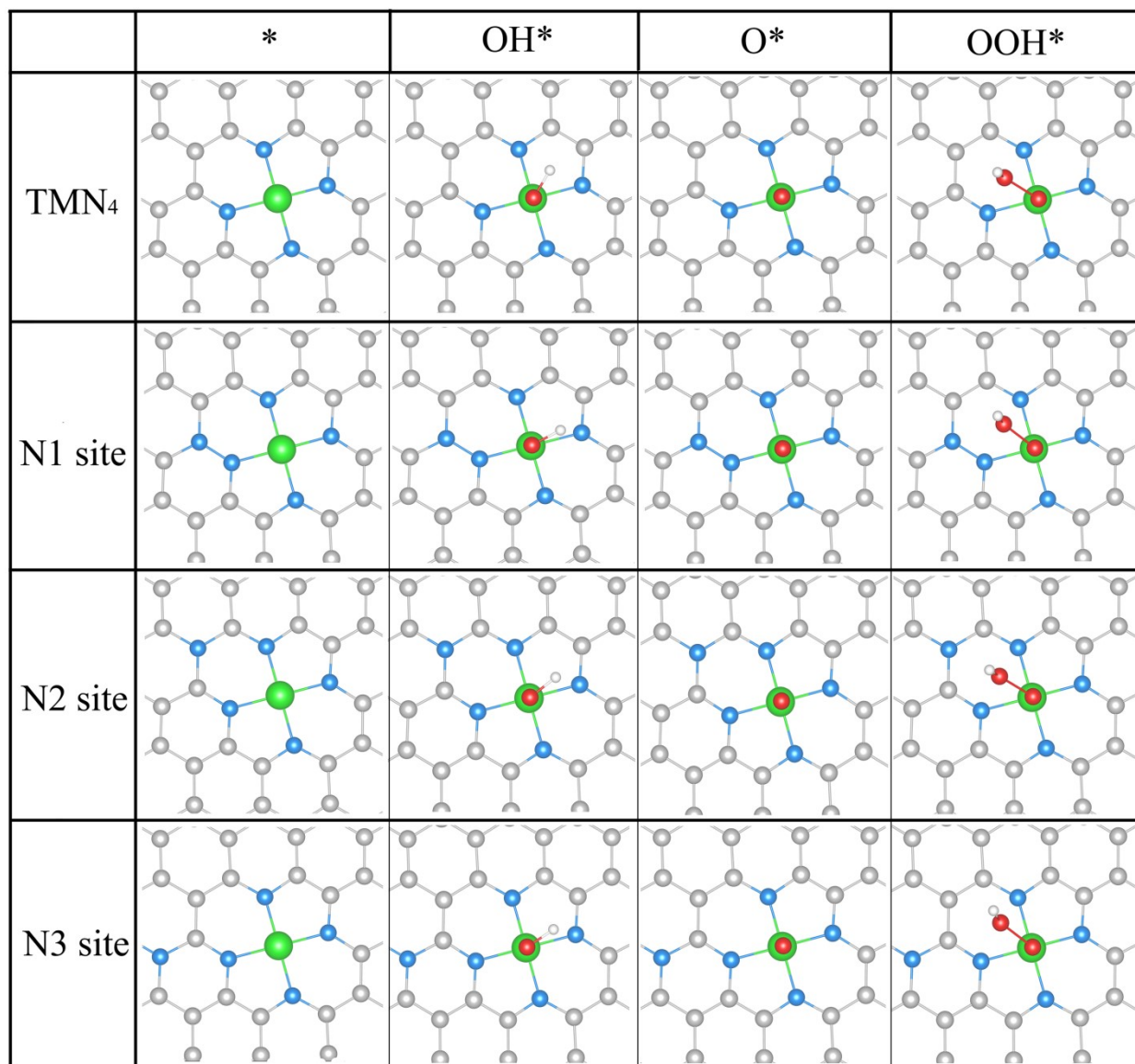


Figure S7. The atom structures of (a) $*$, (b) OH^* , (c) O^* and (d) OOH^* , $*$ denoted the active site of TM monoatom in TM_1 -pyrrolee N_4 systems, where the white, red, gray, blue and green balls denoted the H, O, C, N and TM atoms.

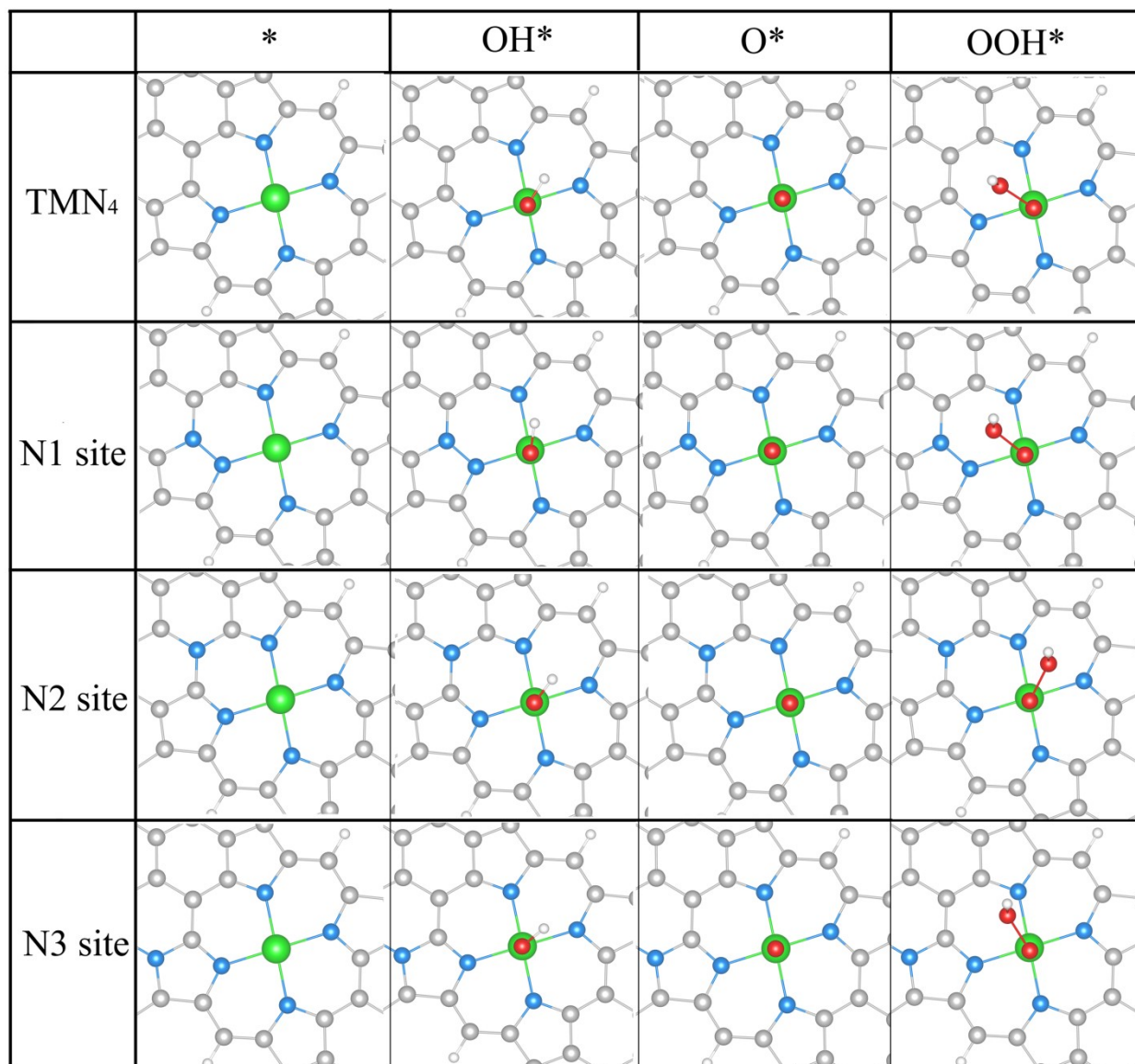


Figure S8. The correlations between the adsorption free energies of OER/ORR oxygenous intermediates and positions of N dopant. The differences of (a) ΔG_{OH^*} , (c) ΔG_{O^*} and (e) ΔG_{OOH^*} between the pristine and N doped TM_1 -pyridine N_4 active centers; The differences of (b) ΔG_{OH^*} , (d) ΔG_{O^*} and (f) ΔG_{OOH^*} between the pristine and N doped TM_1 -pyrrolee N_4 active centers.

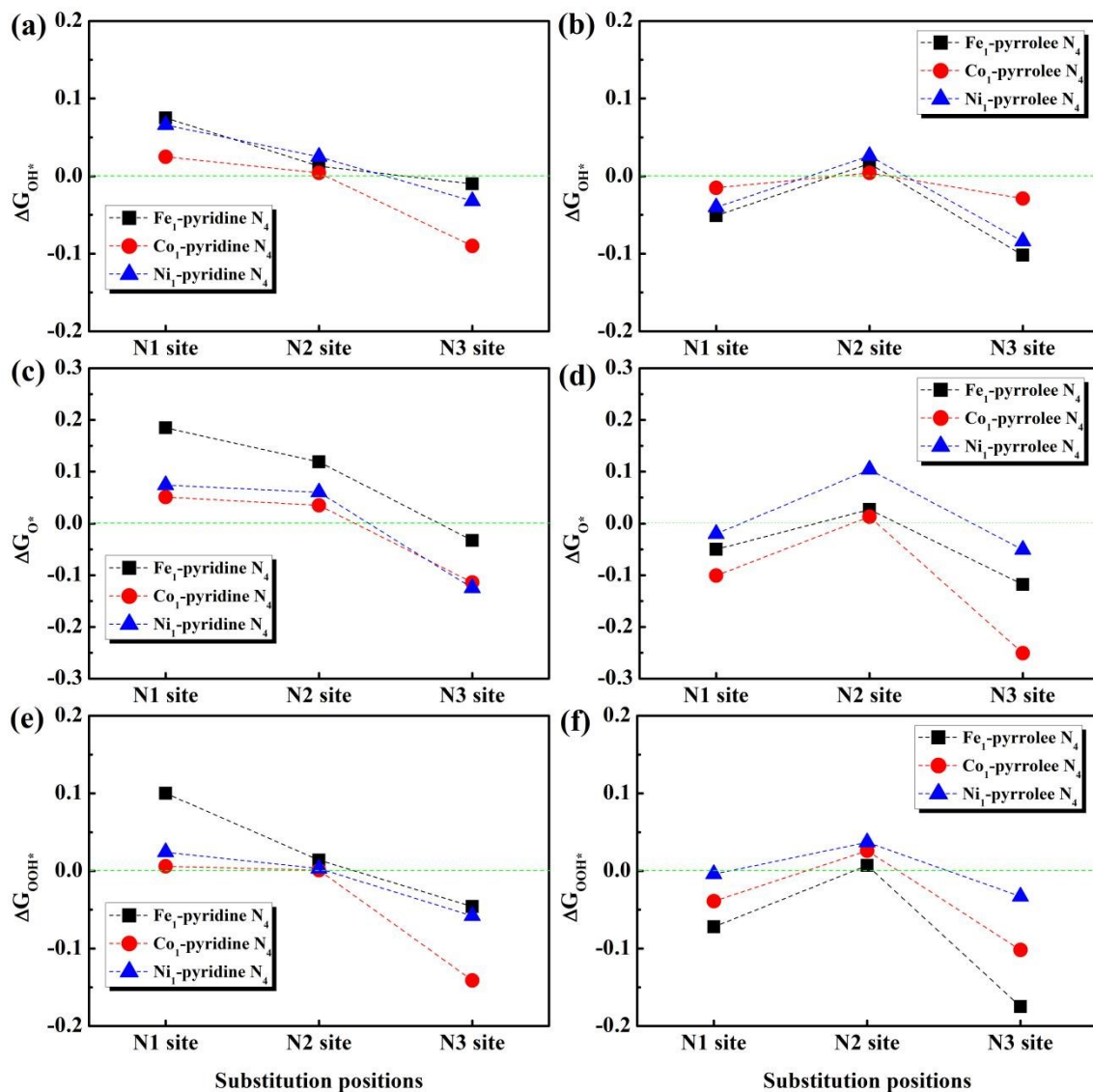


Figure S9. The correlations between the TM_1 (and the first-shell N) atoms and adsorption free energies of (a) ΔG_{OH^*} , (b) ΔG_{O^*} and (c) ΔG_{OOH^*} .

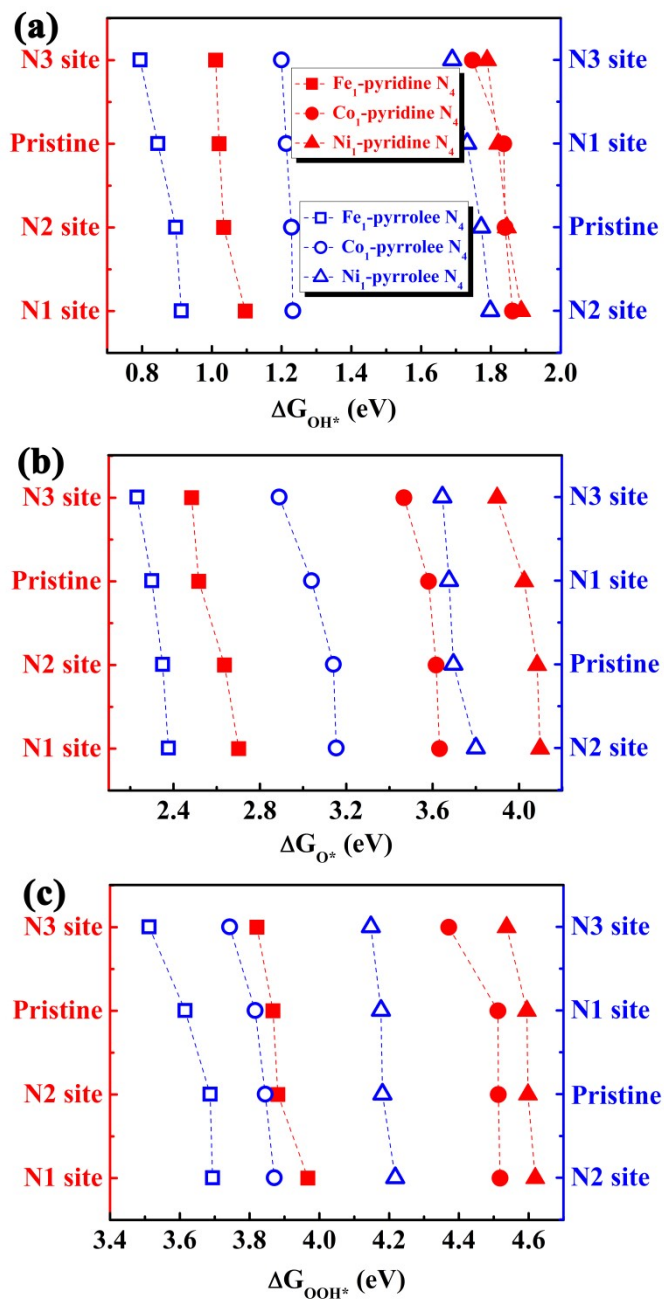


Figure S10. The correlations between the dynamic volume of d electrons (V_d) and adsorption free energies of (a) ΔG_{OH^*} (c) ΔG_{O^*} and (e) ΔG_{OOH^*} .

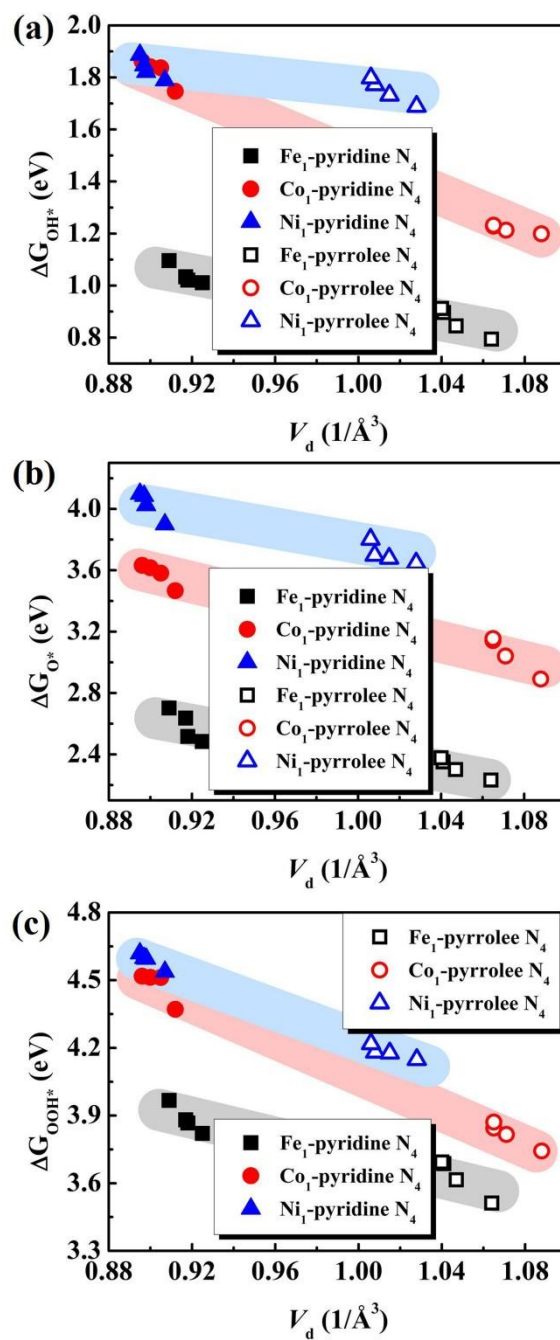
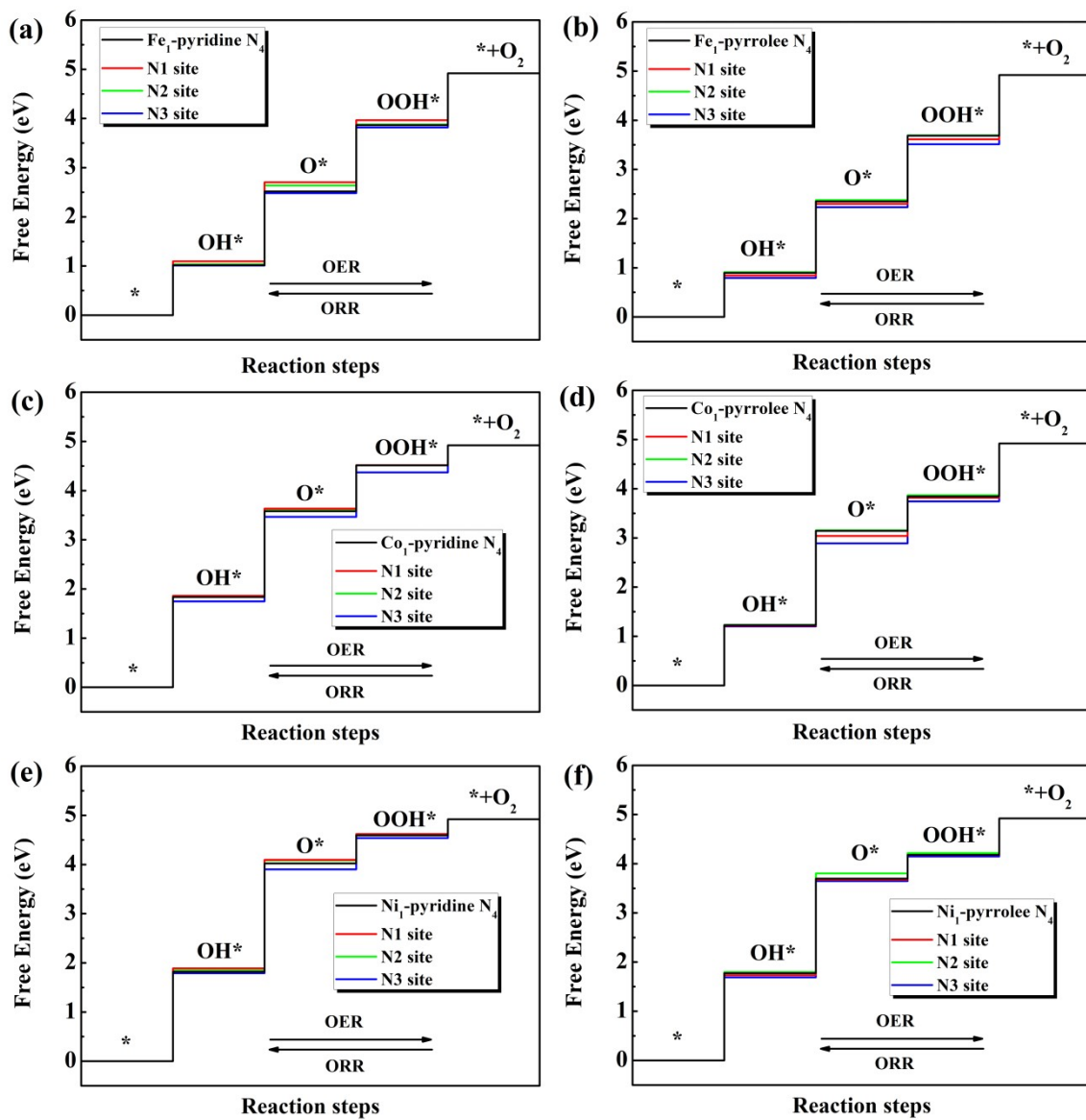


Figure S11. The Gibbs free energy change curves of OER/ORR on the TMN₄ active centers under the potential of U = 0 V. Pristine and N doped (a) Fe₁-pyridine N₄, (b) Fe₁-pyrrolee N₄, (c) Co₁-pyridine N₄, (d) Co₁-pyrrolee N₄, (e) Ni₁-pyridine N₄, (f) Ni₁-pyrrolee N₄ systems.



Data S1. The cartesian coordinate of N3-doped Fe₁-pyrrole N₄.

CIF file

14.3500003815	0.0000000000	0.0000000000
-6.8575266854	12.6054289379	0.0000000000
0.0000000000	0.0000000000	15.0000000000

C	N	H	Fe
53	5	6	1

Direct

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0.300650000	0.866240000	0.103190000
0.357130000	0.979140000	0.103160000
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0.028800000	0.470850000	0.103280000
0.133460000	0.698710000	0.103210000
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0.017210000	0.811570000	0.103190000
0.192680000	0.641610000	0.103380000

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0.473860000	0.197040000	0.103440000
0.139510000	0.529720000	0.103530000
0.308870000	0.525280000	0.102970000
0.130060000	0.869550000	0.103170000
0.188160000	0.811290000	0.103190000
0.869500000	0.130350000	0.103230000
0.811140000	0.188190000	0.103230000
0.742360000	0.742190000	0.103180000
0.635960000	0.364170000	0.103310000
0.305190000	0.694600000	0.103310000
0.364220000	0.635960000	0.103320000
0.694550000	0.304970000	0.103230000
0.253370000	0.352920000	0.100840000
0.258700000	0.258870000	0.100060000
0.197250000	0.474130000	0.103180000
0.654770000	0.547010000	0.103170000
0.453570000	0.345750000	0.102710000
0.547020000	0.654800000	0.103110000
0.345990000	0.453870000	0.101700000
0.974690000	0.857370000	0.103190000
0.025100000	0.142670000	0.103210000
0.856920000	0.974360000	0.103180000
0.142140000	0.025100000	0.103260000
0.816590000	0.816330000	0.103210000
0.184340000	0.185380000	0.098300000
0.500350000	0.500350000	0.102630000

Data S2. The cartesian coordinate of N2-doped Fe₁-pyridine N₄.

CIF file

14.3500003815	0.0000000000	0.0000000000
-7.1750001907	12.4274648747	0.0000000000
0.0000000000	0.0000000000	18.0000000000

C	N	Fe
65	5	1

Direct

0.305860000	0.029820000	0.076900000
0.360020000	0.140870000	0.074550000
0.472850000	0.031770000	0.074760000
0.527090000	0.144020000	0.072240000
0.639330000	0.032480000	0.073590000
0.693760000	0.144410000	0.071810000
0.806120000	0.032530000	0.074740000
0.860820000	0.143760000	0.074000000
0.972220000	0.031140000	0.076500000
0.026760000	0.141800000	0.075990000
0.138760000	0.029870000	0.077370000
0.192600000	0.140230000	0.076020000
0.303340000	0.195330000	0.074180000
0.357410000	0.304750000	0.071320000
0.470640000	0.199830000	0.071660000
0.522120000	0.312470000	0.067780000
0.637950000	0.200730000	0.070070000
0.691540000	0.312880000	0.066640000
0.804880000	0.199430000	0.071820000
0.859740000	0.310380000	0.070250000
0.971440000	0.198010000	0.074690000
0.026780000	0.308940000	0.074000000
0.137150000	0.195590000	0.075440000
0.192230000	0.306380000	0.073960000
0.301570000	0.360410000	0.071900000
0.634740000	0.369990000	0.064620000
0.691980000	0.482500000	0.062370000
0.803410000	0.366200000	0.067130000
0.860230000	0.477120000	0.066560000
0.971360000	0.364840000	0.072320000
0.028720000	0.475820000	0.072920000
0.137750000	0.363010000	0.074170000
0.196680000	0.473670000	0.074300000
0.309270000	0.525140000	0.072650000
0.699040000	0.647480000	0.063990000
0.804410000	0.533560000	0.064020000

0.862880000	0.644270000	0.066510000
0.972510000	0.531480000	0.070630000
0.029640000	0.642210000	0.073000000
0.140870000	0.530050000	0.075100000
0.197750000	0.640930000	0.076480000
0.309960000	0.694550000	0.075910000
0.363060000	0.806280000	0.076330000
0.479660000	0.695000000	0.071170000
0.530190000	0.807220000	0.073000000
0.697970000	0.811510000	0.070850000
0.808650000	0.701420000	0.066560000
0.863980000	0.811290000	0.071470000
0.973840000	0.698290000	0.071450000
0.029570000	0.809010000	0.074990000
0.141400000	0.696750000	0.076510000
0.196320000	0.807850000	0.077800000
0.307340000	0.862730000	0.077520000
0.361830000	0.974420000	0.076690000
0.474100000	0.863030000	0.074880000
0.528510000	0.975540000	0.074500000
0.641220000	0.865380000	0.072880000
0.695450000	0.976750000	0.074070000
0.807810000	0.866280000	0.072810000
0.861650000	0.977020000	0.075340000
0.974020000	0.864990000	0.074880000
0.028420000	0.975740000	0.076930000
0.140440000	0.863690000	0.077590000
0.194940000	0.974440000	0.077860000
0.645780000	0.703400000	0.066700000
0.366980000	0.637710000	0.073260000
0.360080000	0.467680000	0.070220000
0.464720000	0.363680000	0.067890000
0.536530000	0.642440000	0.067380000
0.640630000	0.541360000	0.061910000
0.500980000	0.504640000	0.065610000

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