Supplementary Information (SI) for Physical Chemistry Chemical Physics.
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Supporting Information

Computational high-throughput screening of high-performance transition metal C8N8 single-atom electrocatalysts for oxygen reduction reaction.

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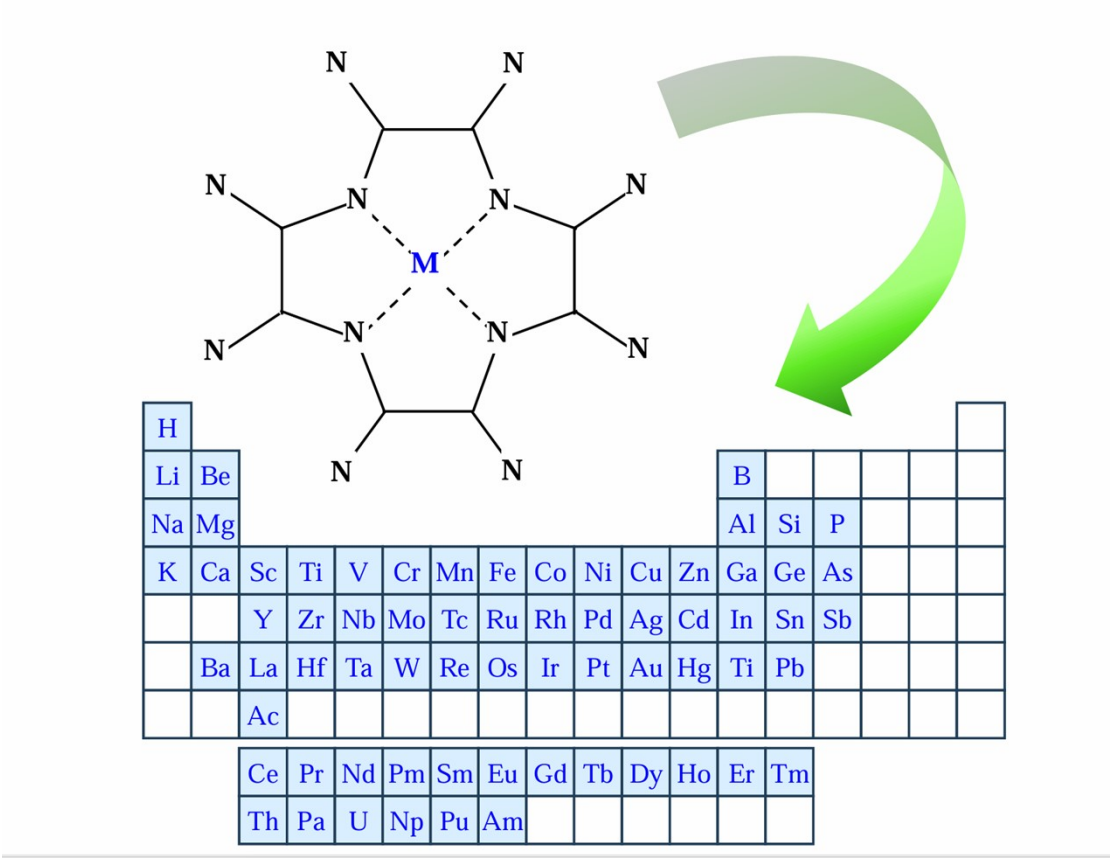
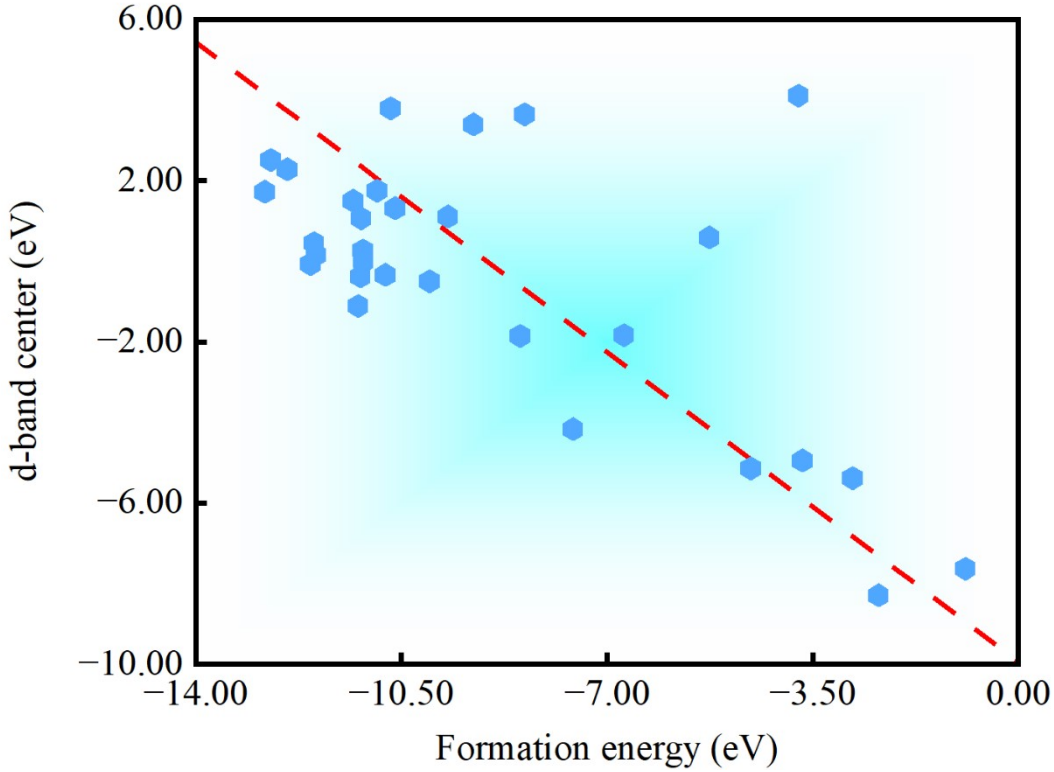


Figure. S2. Linear relationship between formation energy and d-band center.



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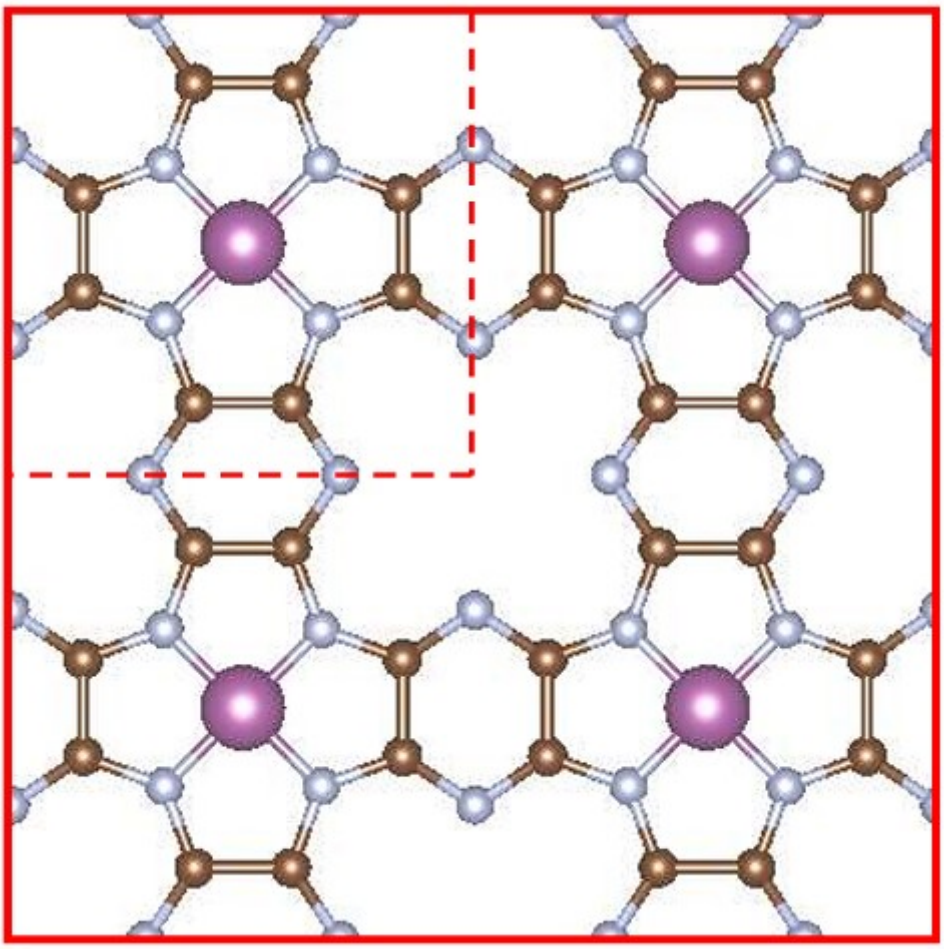

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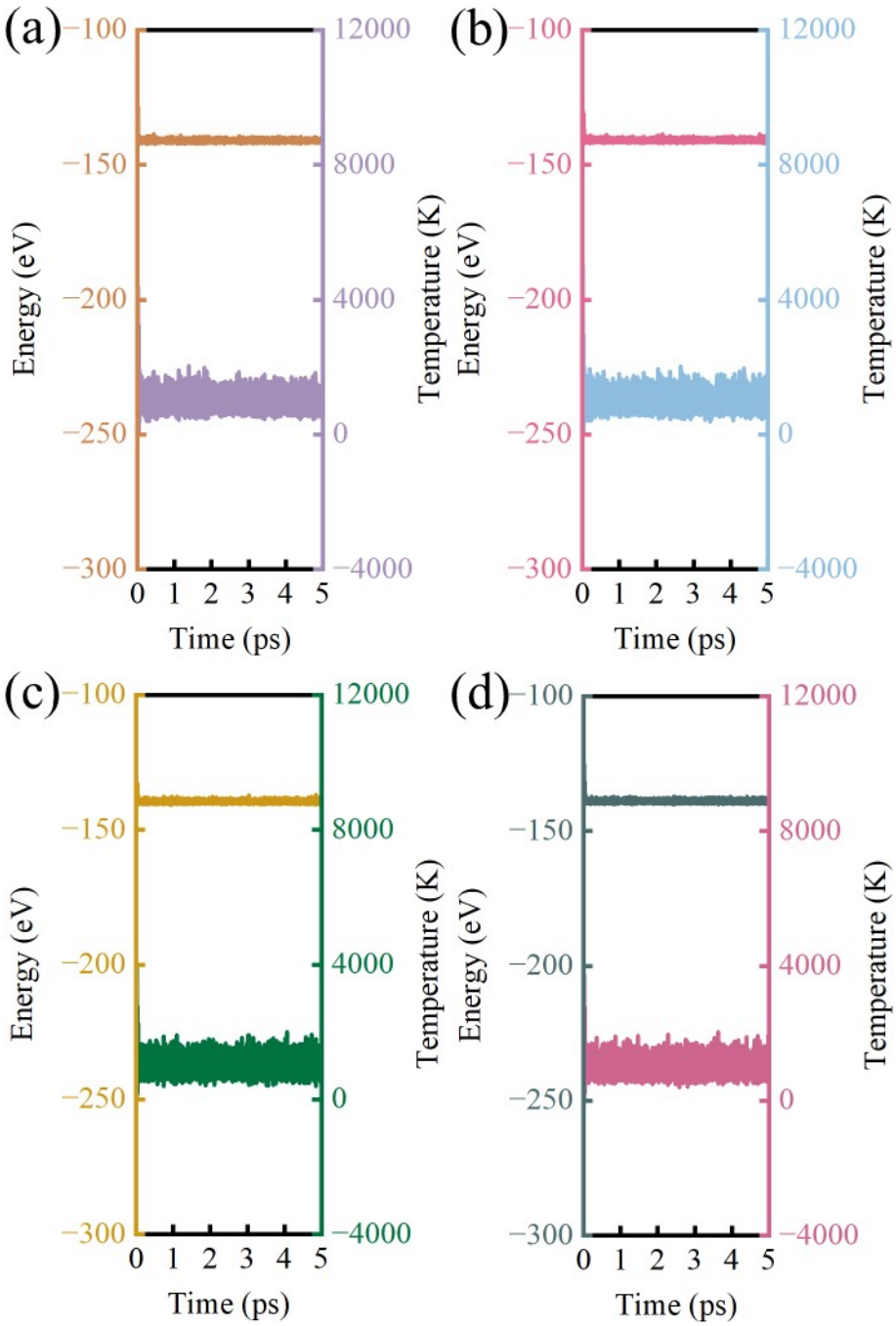

The POSCAR of Fe-C_8N_8.

POSCAR

1.0

7.0798144341	0.0000000000	0.0000000000
0.0000000000	7.0798144341	0.0000000000
0.0000000000	0.0000000000	15.000000000

C N Fe

8 8 1

Direct

0.156021993	0.395461122	0.500000000
0.843977992	0.604538848	0.500000000
0.604538848	0.156021993	0.500000000
0.395461122	0.843977992	0.500000000
0.843977992	0.395461122	0.500000000
0.156021993	0.604538848	0.500000000
0.395461122	0.156021993	0.500000000
0.604538848	0.843977992	0.500000000
0.290396987	0.000000000	0.500000000
0.709602983	0.000000000	0.500000000
0.000000000	0.290396987	0.500000000
0.000000000	0.709602983	0.500000000
0.330963654	0.330963654	0.500000000

0.669036375	0.669036375	0.500000000
0.669036375	0.330963654	0.500000000
0.330963654	0.669036375	0.500000000
0.500000000	0.500000000	0.500000000

The POSCAR of Mn-C_8N_8.

POSCAR

1.0

7.0798144341	0.0000000000	0.0000000000
0.0000000000	7.0798144341	0.0000000000
0.0000000000	0.0000000000	15.000000000

C N Mn

8 8 1

Direct

0.156021993	0.395461122	0.500000000
0.843977992	0.604538848	0.500000000
0.604538848	0.156021993	0.500000000
0.395461122	0.843977992	0.500000000
0.843977992	0.395461122	0.500000000
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0.669036375	0.330963654	0.500000000
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0.500000000	0.500000000	0.500000000

The POSCAR of Co-C_8N_8.

POSCAR

1.0

7.0798144341	0.0000000000	0.0000000000
0.0000000000	7.0798144341	0.0000000000
0.0000000000	0.0000000000	15.000000000

C N Co

8 8 1

Direct

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0.604538848	0.156021993	0.500000000

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0.843977992	0.395461122	0.500000000
0.156021993	0.604538848	0.500000000
0.395461122	0.156021993	0.500000000
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0.709602983	0.000000000	0.500000000
0.000000000	0.290396987	0.500000000
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0.669036375	0.669036375	0.500000000
0.669036375	0.330963654	0.500000000
0.330963654	0.669036375	0.500000000
0.500000000	0.500000000	0.500000000

The POSCAR of Ru-C_8N_8.

POSCAR

1.0

7.0798144341	0.0000000000	0.0000000000
0.0000000000	7.0798144341	0.0000000000
0.0000000000	0.0000000000	15.000000000

C N Ru

8 8 1

Direct

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0.843977992	0.604538848	0.500000000
0.604538848	0.156021993	0.500000000
0.395461122	0.843977992	0.500000000
0.843977992	0.395461122	0.500000000
0.156021993	0.604538848	0.500000000
0.395461122	0.156021993	0.500000000
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0.000000000	0.709602983	0.500000000
0.330963654	0.330963654	0.500000000
0.669036375	0.669036375	0.500000000
0.669036375	0.330963654	0.500000000
0.330963654	0.669036375	0.500000000
0.500000000	0.500000000	0.500000000

(1) The adsorption energies Eads are calculated by the equation.

$$E_{ads} = E_{total} - E_{catalysts} - E_{adsorbates} \#(1)$$

Where $E_{total,}$ $E_{catalysts}$ and $E_{adsorbates}$ represent the energies of the total system after the adsorption, the catalyst, and the adsorbed species, respectively.

(1) The energy of the d band center $E_{d-band\ center}$ can be calculated by the

$$E_{d-band\ center} = \frac{\int E \cdot n(E) dE}{\int n(E) dE} \#(2)$$

following formula:

Where $n(E)$ is the density of states at energy E, and the integration is performed over the entire energy range of the d orbital.

Figure. S5. Based on the Gibbs free energies of adsorbed oxygen-containing intermediates, the scaling relation of $^{\Delta G_{OOH*}}$ vs $^{\Delta G_{OH*}}$.

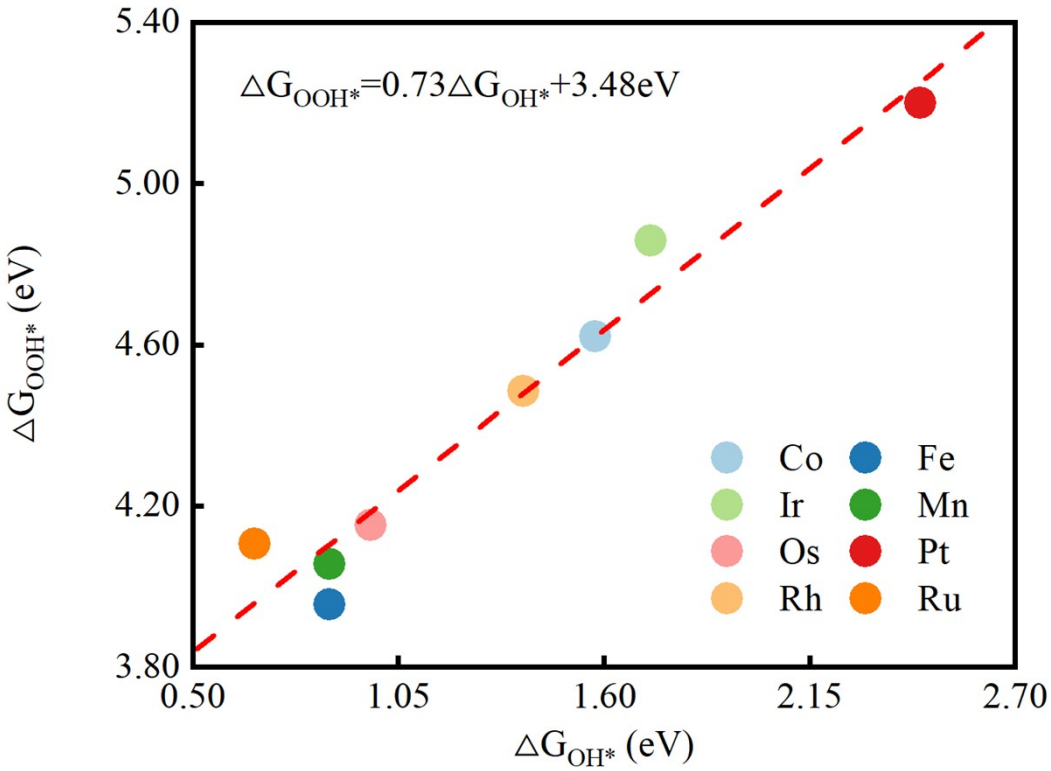

Figure. S6. Schematic of the molecular orbital energy levels of the O_2 molecule.

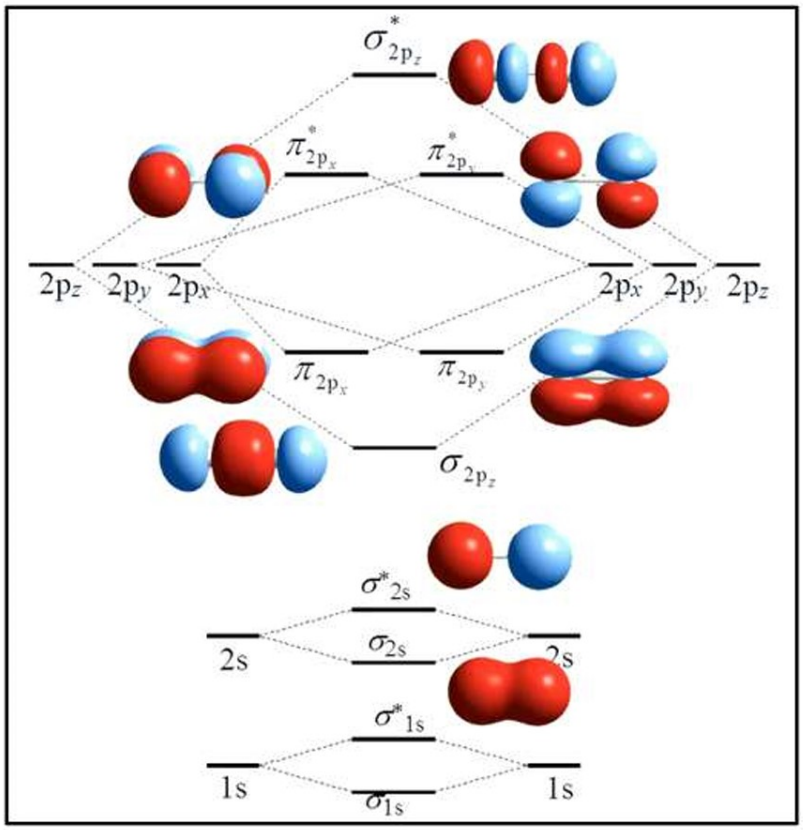

Figure. S7. The major interactions and energy levels of the scalar relativistic Kohn–Sham β-spin of isolated FeO_2 with correlation to the orbitals from Fe and O_2.

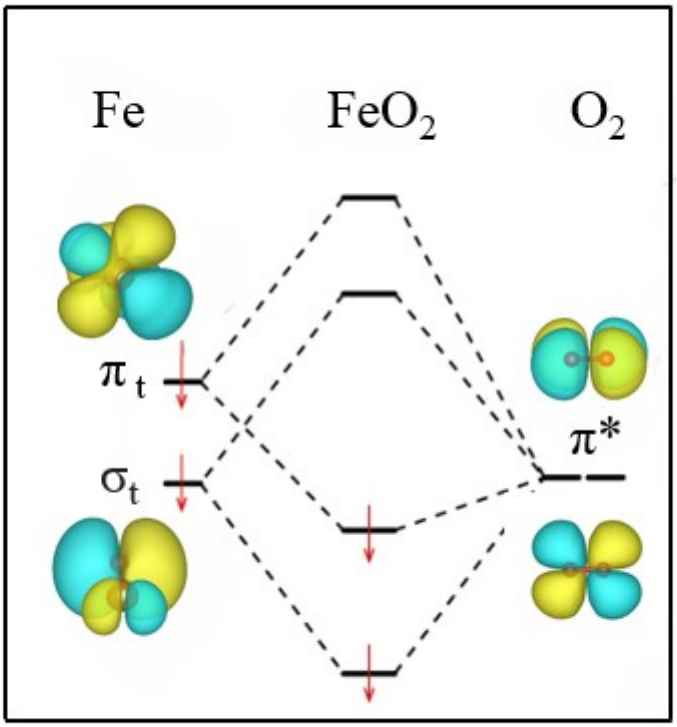

Figure. S8. Schematic interaction of the 3d orbitals of Fe, the 2p orbitals of the O_2 molecule and the projected electronic density of states (PDOS).

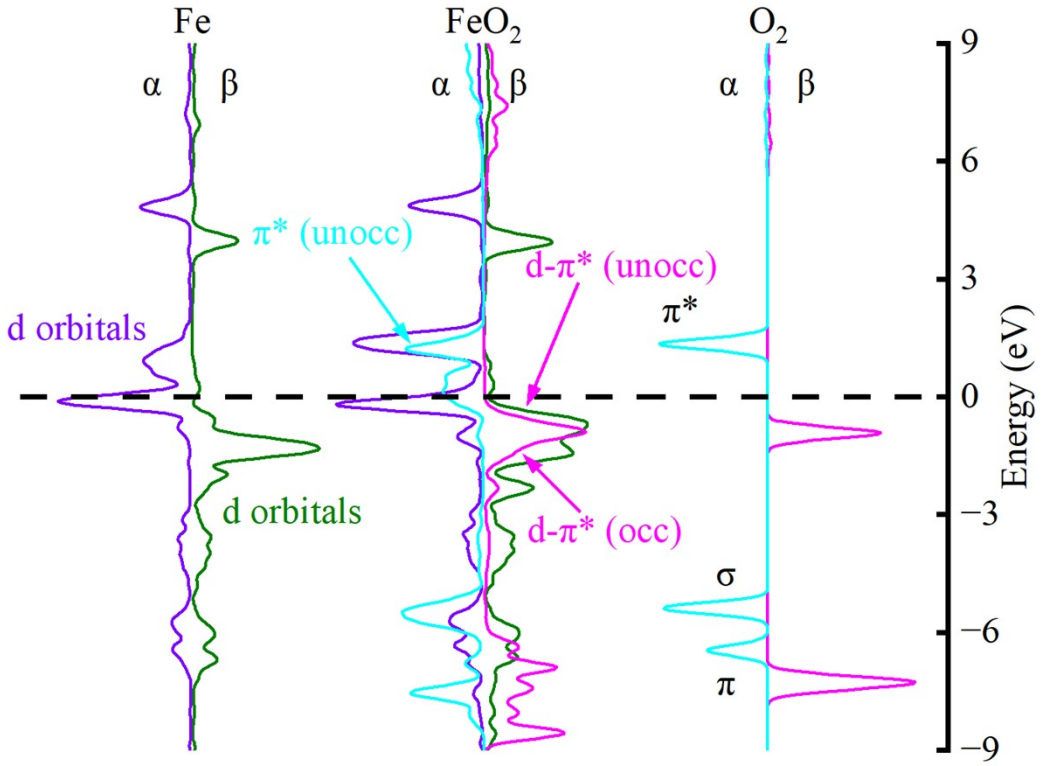

Figure. S9. ENCUT convergence test.

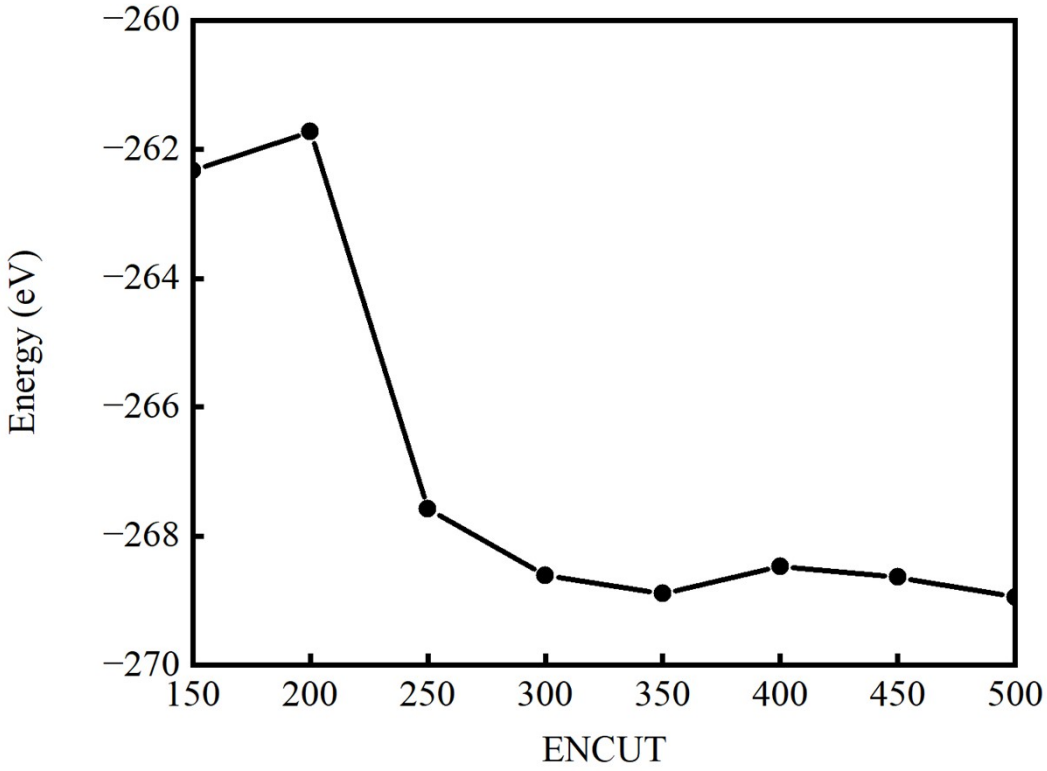

Figure. S10. KPOINTS convergence test**.**

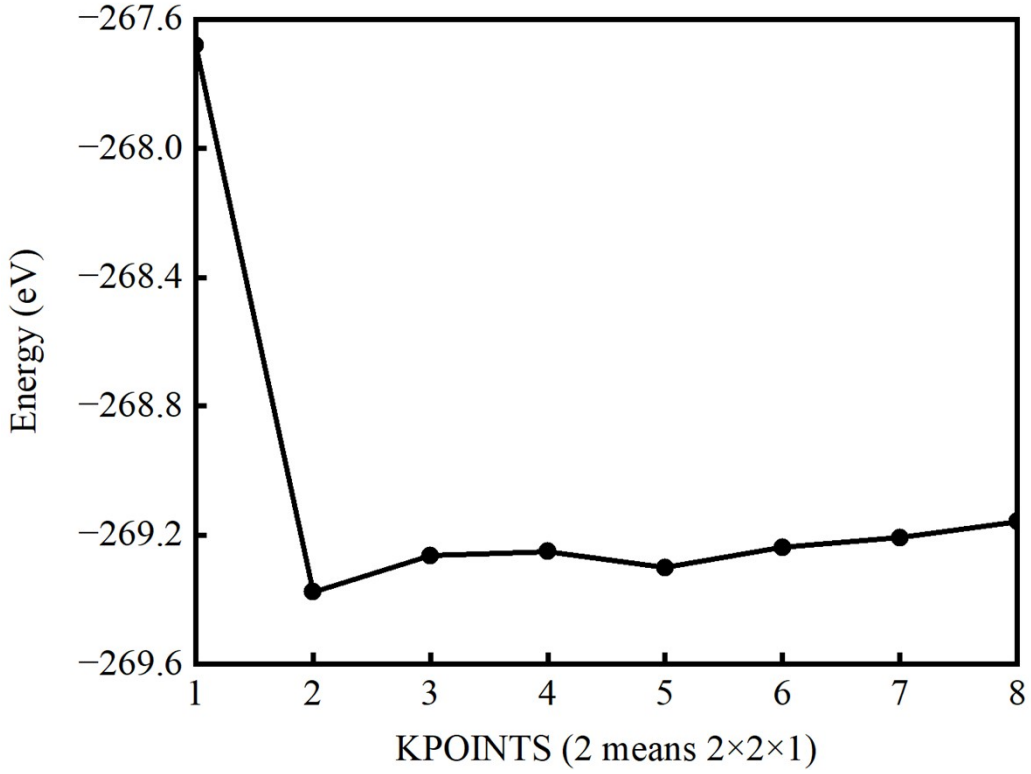

Table S1. Formation energies of TM-C_8N_8 monolayers.

structure	E_a	E_b	E_{atom}	E_f
Sc	-143.24	-132.82	-2.02	-8.40
Ti	-147.93	-132.82	-2.39	-12.72
V	-149.22	-132.82	-3.58	-12.82
Cr	-149.45	-132.82	-5.45	-11.18
Mn	-149.16	-132.82	-5.15	-11.19
Fe	-148.05	-132.82	-3.24	-11.99
Co	-146.71	-132.82	-1.84	-12.05
Ru	-144.34	-132.82	-0.29	-11.23
Cu	-140.64	-132.82	-0.24	-7.58
Zn	-137.38	-132.82	-0.01	-4.55
Y	-138.64	-132.82	-2.08	-3.74
Zr	-144.34	-132.82	-2.25	-9.27
Nb	-146.90	-132.82	-3.18	-10.91
Mo	-147.17	-132.82	-4.65	-9.70
Tc	-147.25	-132.82	-3.28	-11.15
Ru	-145.97	-132.82	-1.21	-11.95
Rh	-144.09	-132.82	-1.26	-10.02
Pd	-141.01	-132.82	-1.48	-6.71
Ag	-135.84	-132.82	-0.20	-2.82
Cd	-133.73	-132.82	-0.01	-0.90

Hf	-146.65	-132.82	-3.15	-10.68
Ta	-148.76	-132.82	-3.50	-12.44
W	-148.71	-132.82	-4.57	-11.31
Re	-148.03	-132.82	-4.61	-10.60
Os	-146.86	-132.82	-2.89	-11.14
Ir	-144.82	-132.82	-1.23	-10.77
Pt	-141.82	-132.82	-0.53	-8.47
Au	-136.68	-132.82	-0.19	-3.67
Hg	-135.21	-132.82	-0.01	-2.38
Rf	-139.20	-132.82	-1.12	-5.26
Db	-139.20	-132.82	-1.12	-5.26
Sg	-139.20	-132.82	-1.12	-5.26
Bh	-139.20	-132.82	-1.12	-5.26
Hs	-139.20	-132.82	-1.12	-5.26
Mt	-139.20	-132.82	-1.12	-5.26
Ds	-139.20	-132.82	-1.12	-5.26
Rg	-139.20	-132.82	-1.12	-5.26
Cn	-139.20	-132.82	-1.12	-5.26

Table S2. Adsorption energies of single O molecule on TM-C_8N_8 monolayers

structure	E_{total}	$E_{catalysts}$	$E_{adsorbates}$	E_{ads}
Sc	-147.77	-143.24	-1.54	-2.62
Ti	-154.89	-147.93	-1.54	-4.98
V	-156.58	-149.22	-1.54	-5.38
Cr	-156.40	-149.45	-1.54	-4.96
Mn	-155.37	-149.16	-1.54	-4.22
Fe	-153.03	-148.05	-1.54	-3.00
Co	-150.54	-146.71	-1.54	-1.88
Ni	-146.83	-144.34	-1.54	-0.57
Cu	-142.88	-140.64	-1.54	-0.32
Zn	-139.67	-137.38	-1.54	-0.36
Y	-143.27	-138.64	-1.54	-2.74
Zr	-151.40	-144.34	-1.54	-5.10
Nb	-155.04	-146.90	-1.54	-6.16
Mo	-155.09	-147.17	-1.54	-5.94
Tc	-154.65	-147.25	-1.54	-5.41
Ru	-151.92	-145.97	-1.54	-3.97
Rh	-148.50	-144.09	-1.54	-2.45
Pd	-143.69	-141.01	-1.54	-0.75
Ag	-137.94	-135.84	-1.54	-0.26
Cd	-138.01	-133.73	-1.54	-2.33

Hf	-153.94	-146.65	-1.54	-5.32
Ta	-156.93	-148.76	-1.54	-6.19
W	-156.48	-148.71	-1.54	-5.79
Re	-155.22	-148.03	-1.54	-5.19
Os	-152.82	-146.86	-1.54	-3.99
Ir	-149.32	-144.82	-1.54	-2.54
Pt	-144.77	-141.82	-1.54	-1.02
Au	-138.79	-136.68	-1.54	-0.22
Hg	-137.63	-135.21	-1.54	-0.53
Rf	-140.49	-139.20	-1.54	0.63
Db	-140.49	-139.20	-1.54	0.63
Sg	-140.49	-139.20	-1.54	0.63
Bh	-140.49	-139.20	-1.54	0.63
Hs	-140.49	-139.20	-1.54	0.63
Mt	-140.49	-139.20	-1.54	0.63
Ds	-140.49	-139.20	-1.54	0.63
Rg	-140.49	-139.20	-1.54	0.63
Cn	-140.49	-139.20	-1.54	0.63

Table S3. Comparison of the Calculated ORR Electrocatalytic Performance of TM-C_8N_8 Materials with Experimental Data of TM-PC Materials.

structure	ΔG_{O*}	ΔG_{OH*}	ΔG_{OOH*}	η_{ORR}
Fe- C_8N_8 (theory)	2.16	0.87	3.96	0.26
Fe-Pc$_{(experiment)}$	**1.65**	**1.00**	**3.91**	**0.54**
Mn- C_8N_8 (theory)	1.76	0.87	4.06	0.36
Mn-Pc$_{(experiment)}$	**1.65**	**1.03**	**4.05**	**0.56**
Co- C_8N_8 (theory)	3.46	1.58	4.62	0.93
Co-Pc$_{(experiment)}$	**3.13**	**1.40**	**4.27**	**0.58**
Ru- C_8N_8 (theory)	1.96	0.67	4.11	0.42
Ru-Pc$_{(experiment)}$	**4.49**	**2.38**	**5.11**	**1.42**