Electronic supplementary information

Dual-metal atoms incorporated N-doped graphenes as the oxygen evolution reaction electrocatalysts: high activities achieved by site synergies †

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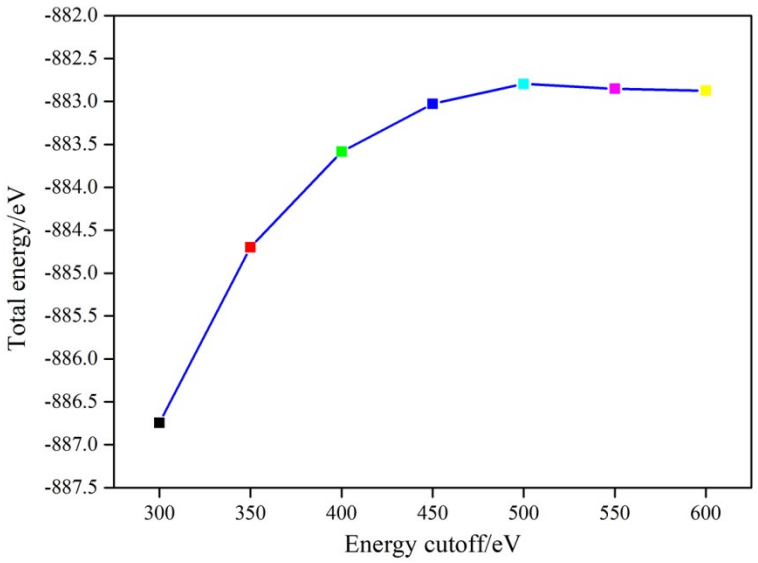


Fig. S1 Calculated total energies of $CoCoN_6$-gra using different energy cutoff values.

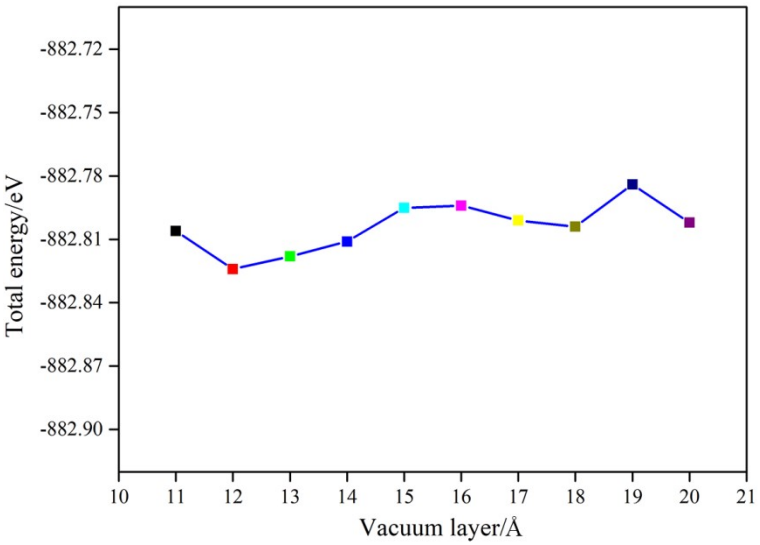


Fig. S2 Calculated total energies of $CoCoN_6$-gra as a function of the thickness of vacuum layer (11-20 Å).

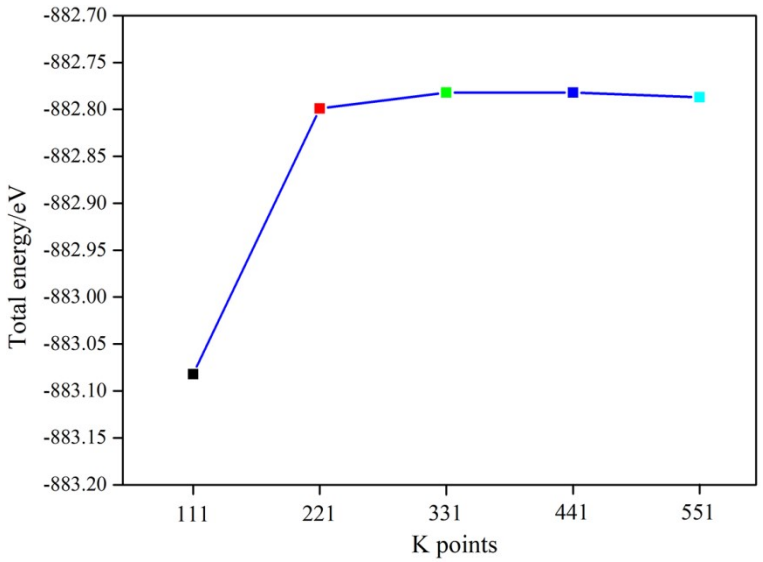


Fig. S3 Calculated total energies of $CoCoN_6$-gra using different *k*-point meshes.

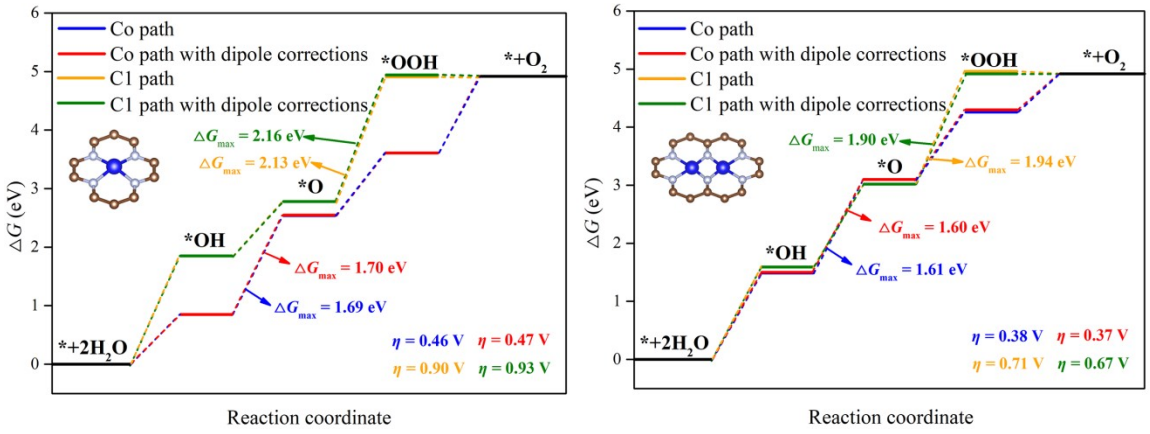


Fig. S4 Gibbs free energy diagrams for the single-site OER mechanism on CoN_4-gra and $CoCoN_6$-gra with and without dipole corrections. C1 atom is shown in Fig. 1 of main text. According to the small difference, the corrections were not considered in the current work.

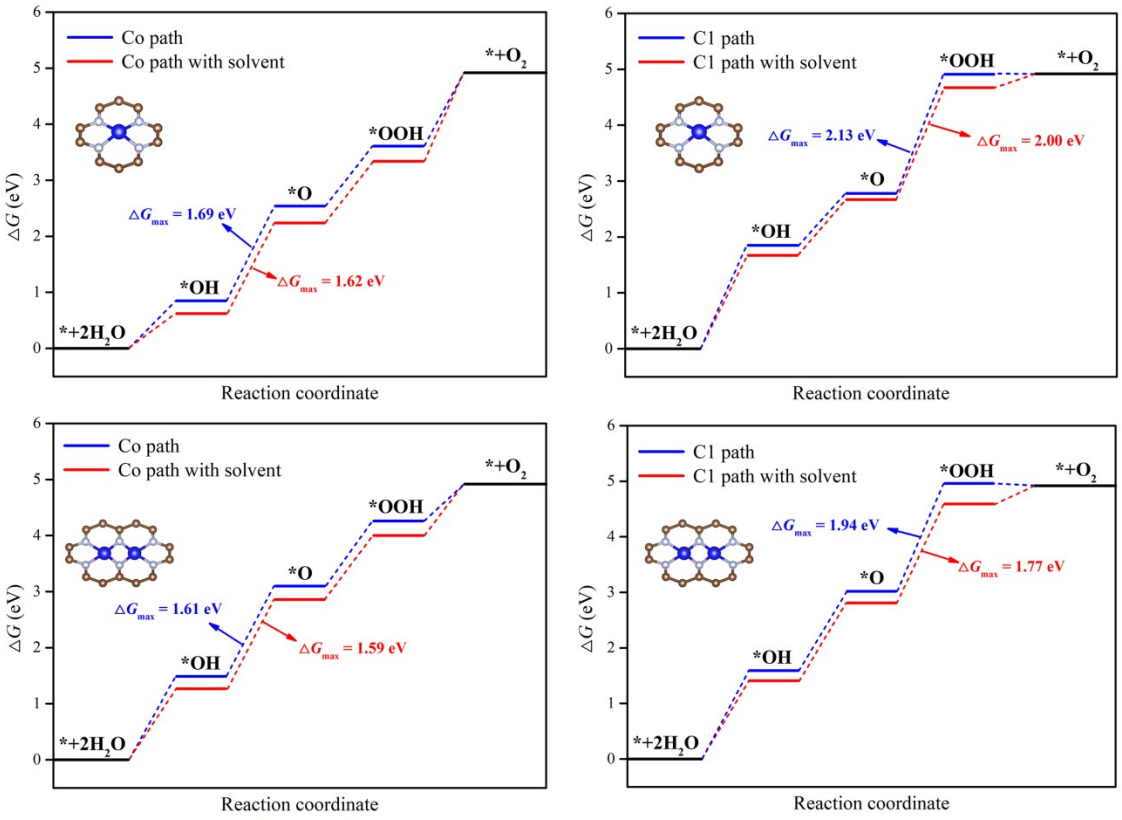


Fig. S5 Gibbs free energy diagrams for the single-site OER mechanism on CoN_4-gra (upper) and $CoCoN_6$-gra (down) with and without solvent. C1 atom is shown in Fig. 1 of main text. According to the same change trend for all intermediates, the corrections were not considered in the current work.

Table S1 The average distances ($d_{M\text{-}N}$, Å) vs. sum of covalent radii ($r_M + r_N$, Å) of the metal and N atoms, and the distances ($d_{M\text{-}M}$, Å) vs. sum of covalent radii ($r_M + r_M$, Å) of two adjacent metal atoms.

Model	$d_{M\text{-}N}$	$r_M + r_N$	$d_{M\text{-}M}$	$r_M + r_M$
FeN_4-gra	1.89	2.38	-	-
CoN_4-gra	1.88	1.97	-	-
NiN_4-gra	1.87	1.88	-	-
$FeFeN_6$-gra	1.87	2.38	2.25	3.34
$CoCoN_6$-gra	1.85	1.97	2.25	2.52
$NiNiN_6$-gra	1.85	1.88	2.56	2.34
$FeCoN_6$-gra	1.86/1.86	2.38/1.97	2.25	2.93
$FeNiN_6$-gra	1.86/1.86	2.38/1.88	2.43	2.84
$CoNiN_6$-gra	1.85/1.86	1.97/1.88	2.41	2.43

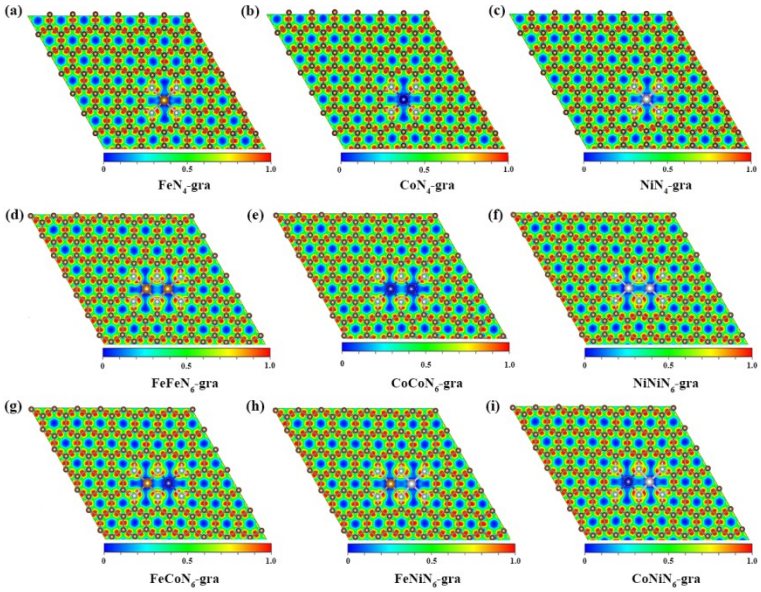


Fig. S6 Electron localization functions (ELFs) for the N-doped graphene planes of all the catalysts shown in Fig. 1 of main text.

Table S2 Formation energies (E_f, eV) calculated using pure graphene and nitrogen as references.

Model	E_f
FeN_4-gra	-3.62
CoN_4-gra	-4.08
NiN_4-gra	-3.56
$FeFeN_6$-gra	-8.49
$CoCoN_6$-gra	-8.66
$NiNiN_6$-gra	-7.25
$FeCoN_6$-gra	-8.62
$FeNiN_6$-gra	-7.61
$CoNiN_6$-gra	-7.78

$$E_f = E_{MN4\text{-}gra} - n_C \cdot E_C - E_M - n_N \cdot E_N$$

$$E_f = E_{MMN6\text{-}gra} - n_C \cdot E_C - n_M \cdot E_M - n_N \cdot E_N$$

$$E_f = E_{M1M2N6\text{-}gra} - n_C \cdot E_C - E_{M1} - E_{M2} - n_N \cdot E_N$$

whereas $E_{MN4\text{-}gra}$, $E_{MMN6\text{-}gra}$ and $E_{M1M2N6\text{-}gra}$ are the total energies of the MN_4-gra, MMN_6-gra and $M1M2N_6$-gra, respectively; n_C, n_N and n_M are the atom numbers of C, N, and metal atoms in the catalyst model, respectively. E_C and E_N are the energies of a carbon

atom in pure graphene and the half of a free N_2 molecule, respectively. E_M is the energy of the isolated M atom according to the literature.[S1]

Table S3 Standard dissolution potentials (U^0_{diss}) of metal atoms, number of transferred electrons (n) during the dissolution, and calculated dissolution potentials (U_{diss}, V vs. SHE) of the metals in various catalysts.

Model	U°_{diss}	n	U_{diss}
FeN_4-gra	-0.45	2	0.70
CoN_4-gra	-0.28	2	1.03
NiN_4-gra	-0.26	2	0.87
$FeFeN_6$-gra	-0.45	2	1.41
$CoCoN_6$-gra	-0.28	2	1.55
$NiNiN_6$-gra	-0.26	2	1.10
$FeCoN_6$-gra	-0.45/-0.28	2/2	1.21/1.31
$FeNiN_6$-gra	-0.45/-0.26	2/2	1.08/0.71
$CoNiN_6$-gra	-0.28/-0.26	2/2	1.26/0.79

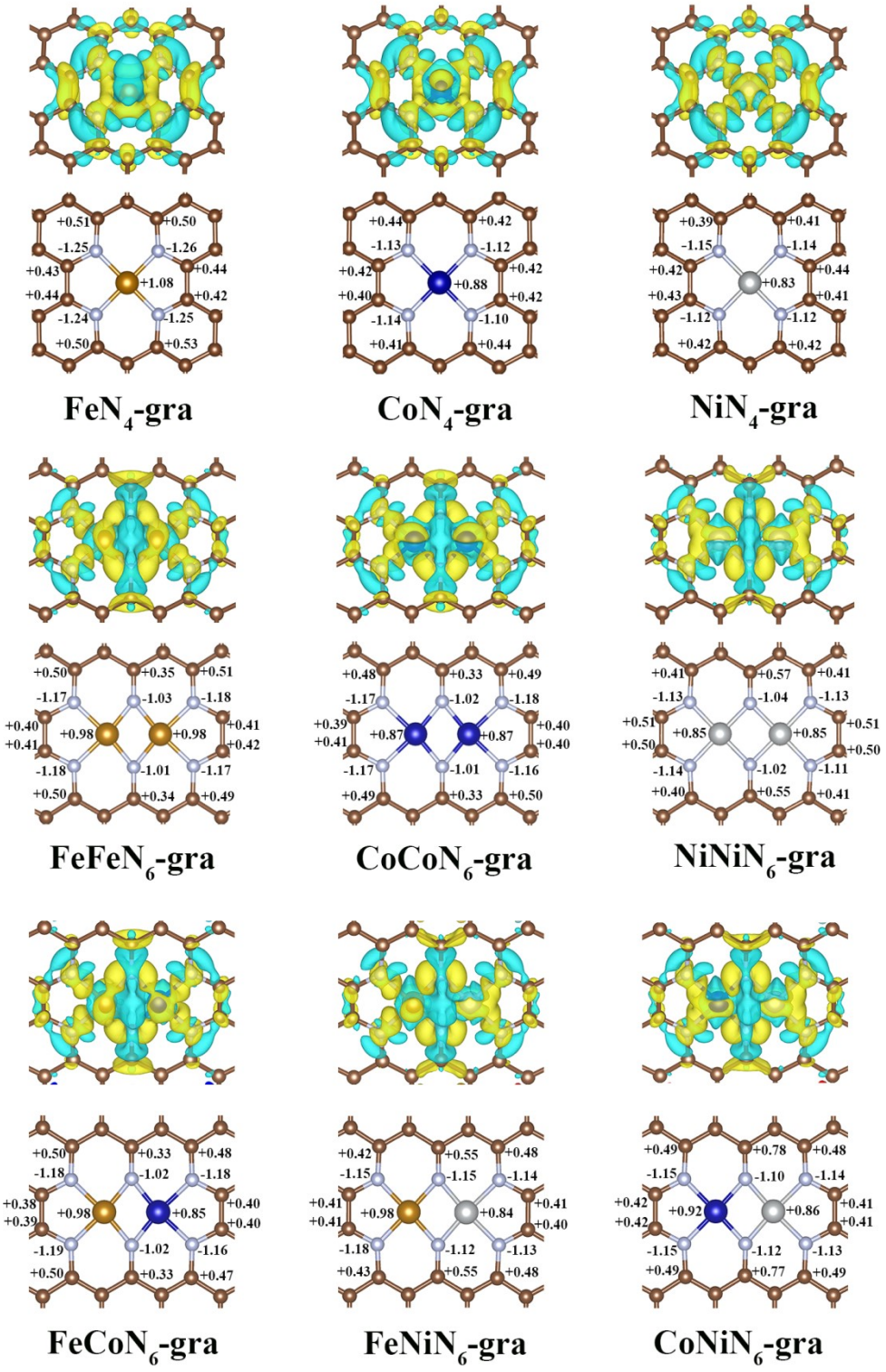


Fig. S7 Charge density difference plot (upper) and calculated Bader charges (down) for each catalyst. The yellow and cyan colors denote the electron accumulation and depletion, respectively. The charge density difference was calculated as follows.

$$\Delta\rho(\mathrm{r}) = \rho(\mathrm{r})_{\mathrm{MN4\text{-}gra}} - \rho(\mathrm{r})_{\mathrm{M}} - \rho(\mathrm{r})_{\mathrm{N4\text{-}gra}}$$

$$\Delta\rho(r) = \rho(r)_{MMN6\text{-}gra} - \rho(r)_{MM} - \rho(r)_{N6\text{-}gra}$$

$$\Delta\rho(r) = \rho(r)_{M1M2N6\text{-}gra} - \rho(r)_{M1M2} - \rho(r)_{N6\text{-}gra}$$

where $\rho(r)_{MN4\text{-}gra}$, $\rho(r)_{MMN6\text{-}gra}$ and $\rho(r)_{M1M2N6\text{-}gra}$ are the charge density of the catalysts, $\rho(r)_{N4\text{-}gra}$ and $\rho(r)_{N6\text{-}gra}$ are the charge density of the catalysts without metals, and $\rho(r)_{M}$, $\rho(r)_{MM}$ and $\rho(r)_{M1M2}$ are the charge density of the metal atoms.

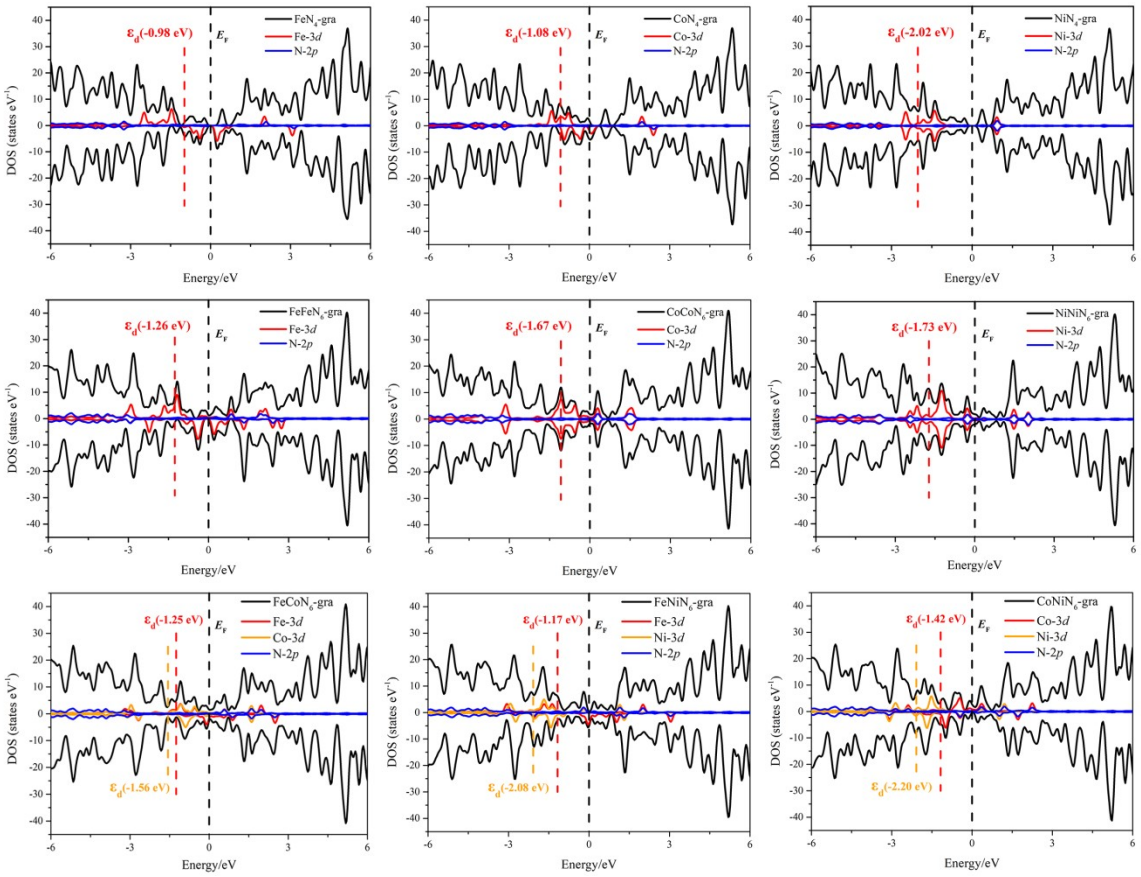


Fig. S8 Total DOSs and projected M-3*d* and N-2*p* states of all catalysts with the metal d-band centers (ε_d) calculated from both spin up and spin down states. Fermi levels are set at 0 eV.

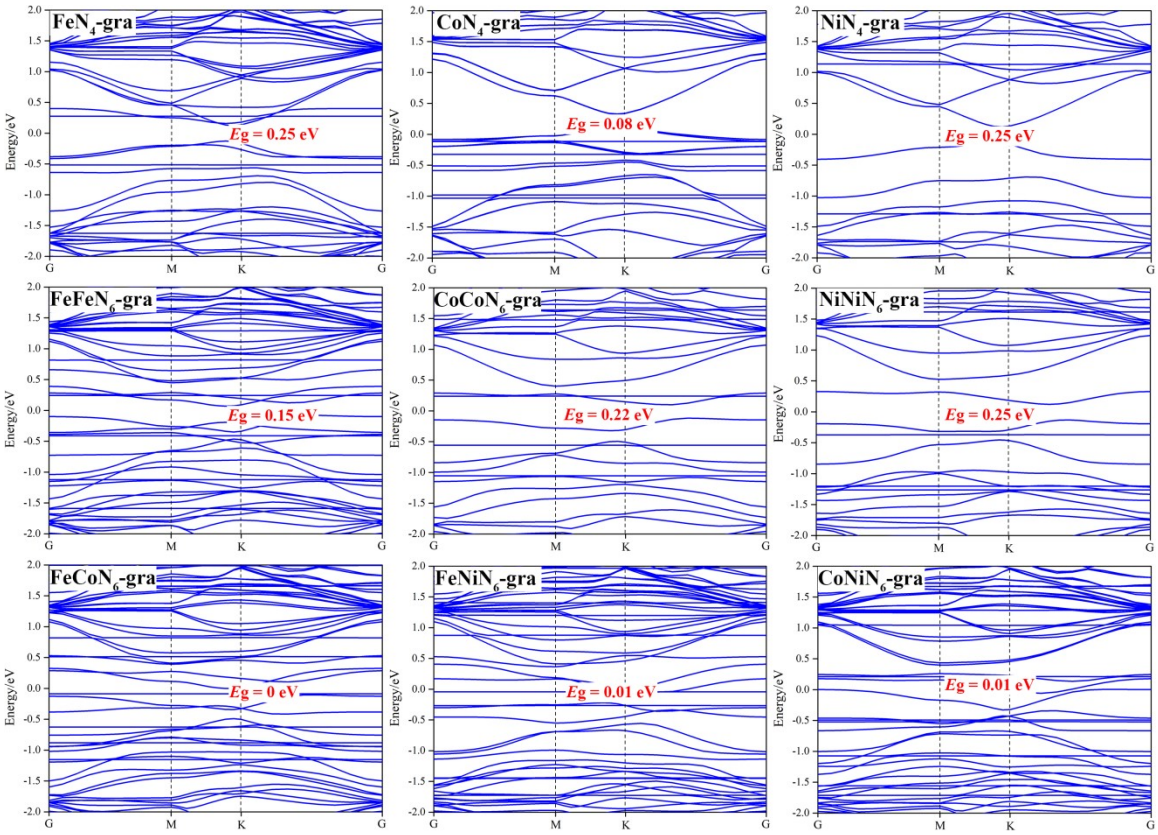


Fig. S9 Electronic band structures of catalysts.

Table S4 Optimized adsorption structures (distance unit: Å) and adsorption free energies of reaction intermediates involved in single-site OER mechanism on different active sites of FeN_4-gra.

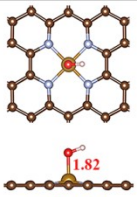
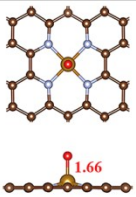
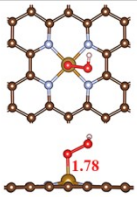
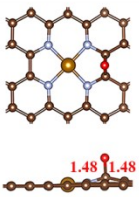
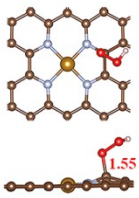
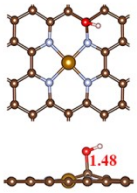
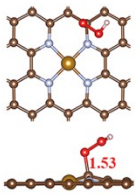
FeN_4-gra	*OH	*O	*OOH
Fe site	 0.47 eV	 1.22 eV	 3.24 eV
C1 site	 1.88 eV	 2.69 eV	 4.93 eV
C2 site	 2.08 eV	 3.06 eV	 5.09 eV

Table S5 Optimized adsorption structures (distance unit: Å) and adsorption free energies of reaction intermediates involved in single-site OER mechanism on different active sites of CoN_4-gra.

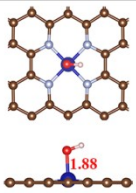
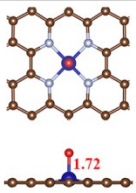
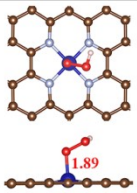
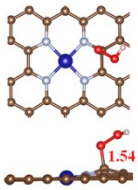
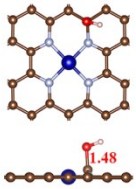
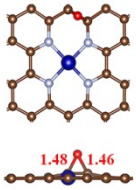
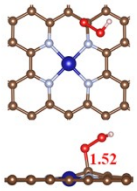
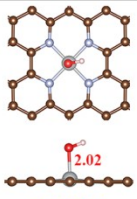
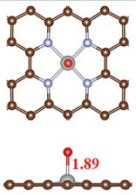
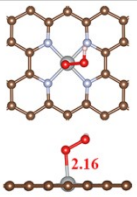
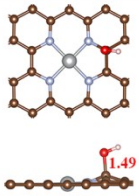
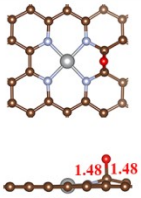
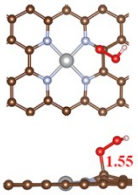
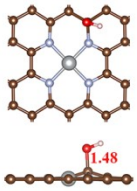
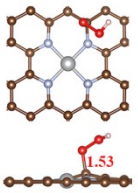
CoN_4-gra	*OH	*O	*OOH
Co site	 0.85 eV	 2.54 eV	 3.61 eV
C1 site	 1.85 eV	 2.78 eV	 4.91 eV
C2 site	 2.10 eV	 3.08 eV	 5.12 eV

Table S6 Optimized adsorption structures (distance unit: Å) and adsorption free energies of reaction intermediates involved in single-site OER mechanism on different active sites of NiN_4-gra.

NiN_4-gra	*OH	*O	*OOH
Ni site	 1.92 eV	 4.18 eV	 4.57 eV
C1 site	 2.00 eV	 2.91 eV	 5.04 eV
C2 site	 2.10 eV	 3.13 eV	 5.12 eV

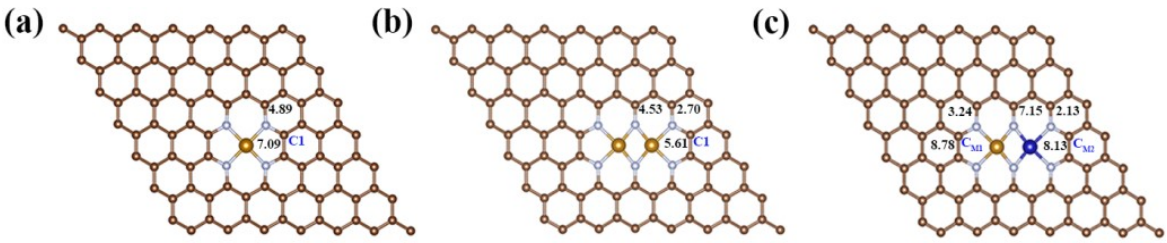


Fig. S10 Calculated NICS value (ppm) for each carbon sites around the metal centers for FeN_4-gra, $FeFeN_6$-gra and $FeCoN_6$-gra as representatives. A more positive NICS value suggests more antiaromatic character of the site. The calculations were carried out using the PBE functional with the 6-31G* basis set for the nonmetal atoms and Stuttgart/Dresden quasirelativistic effective core potential (ECP) and the corresponding basis set for metals, as implemented in the Gaussian 16 software package.[S2]

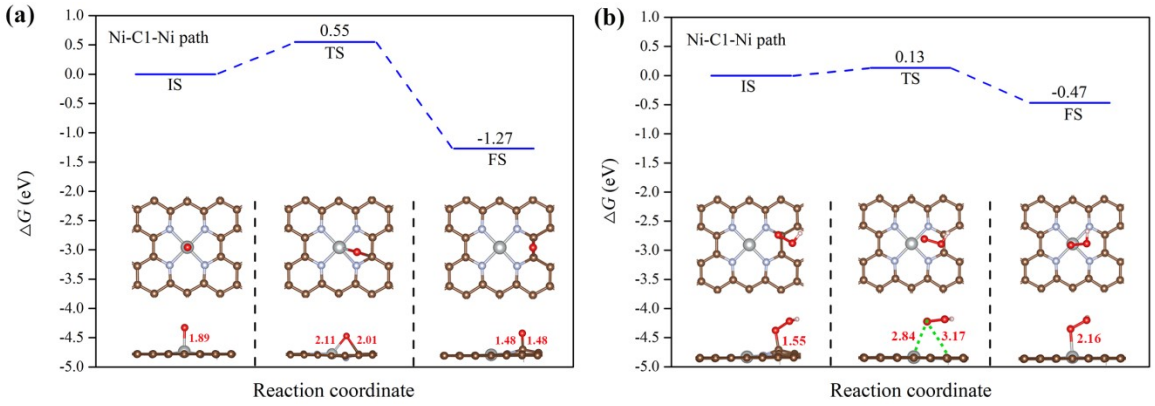


Fig. S11 Calculated free energy barriers for (a) O transfers from the Ni to C1 site; (b) OOH transfers from the C1 to Ni site of NiN_4-gra using the NEB method. IS, TS, and FS denote the initial state, transition state and final state, respectively.

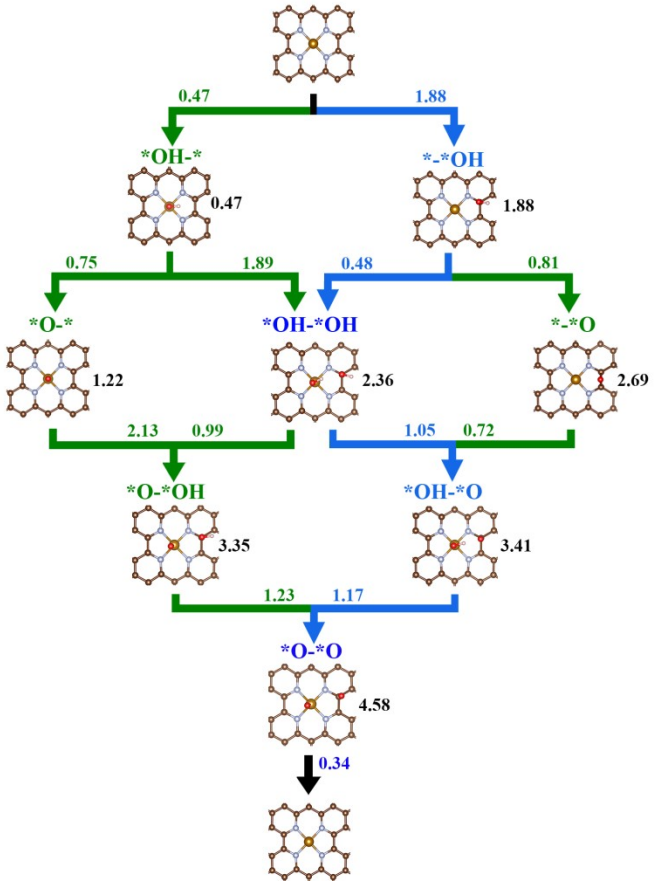


Fig. S12 Calculated free energy changes (eV) for the dual-site *O-*O coupling mechanism on FeN_4-gra. Adsorption free energies of corresponding intermediates are given in black. Blue arrows represent the energetically most favorable path. An adsorption intermediate is named according to its exact adsorption position on the two active sites. For instance, *OH-* and *-*OH represent the OH adsorbed at the left metal and right C1 site, respectively.

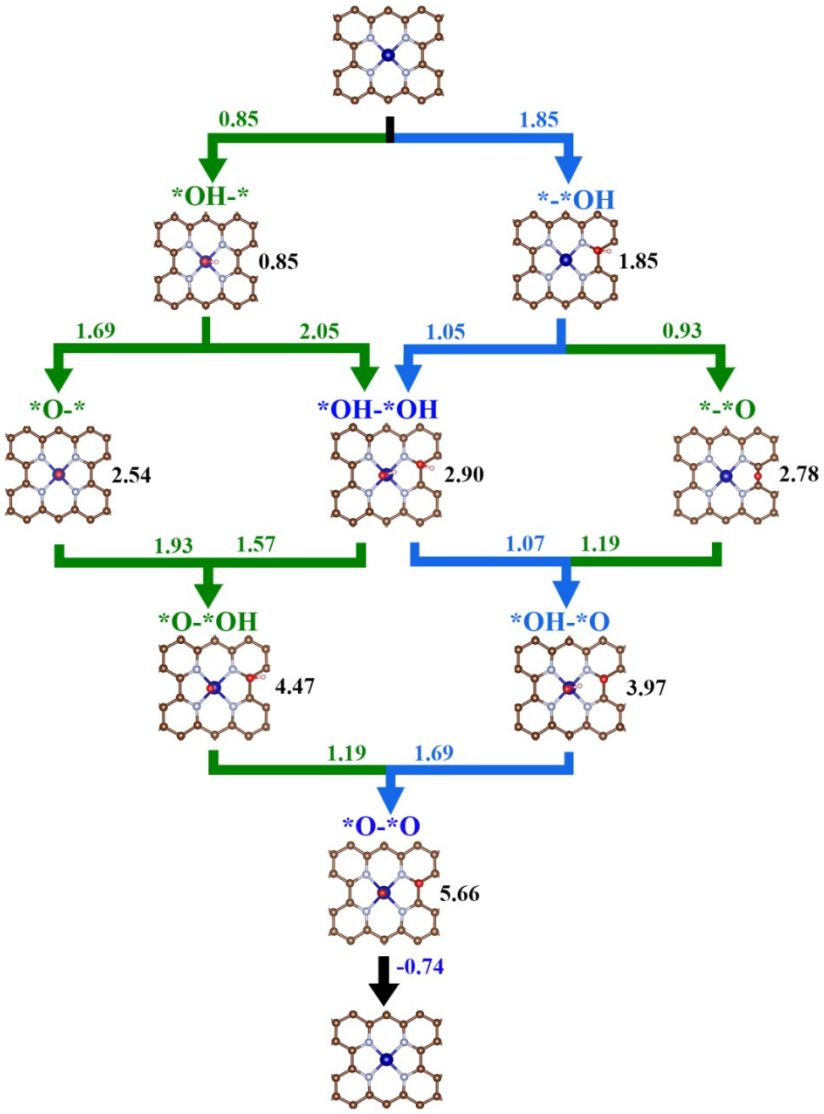


Fig. S13 Calculated free energy changes (eV) for dual-site *O-*O coupling mechanism on CoN_4-gra. Adsorption free energies of corresponding intermediates are given in black. Blue arrows represent the energetically most favorable path.

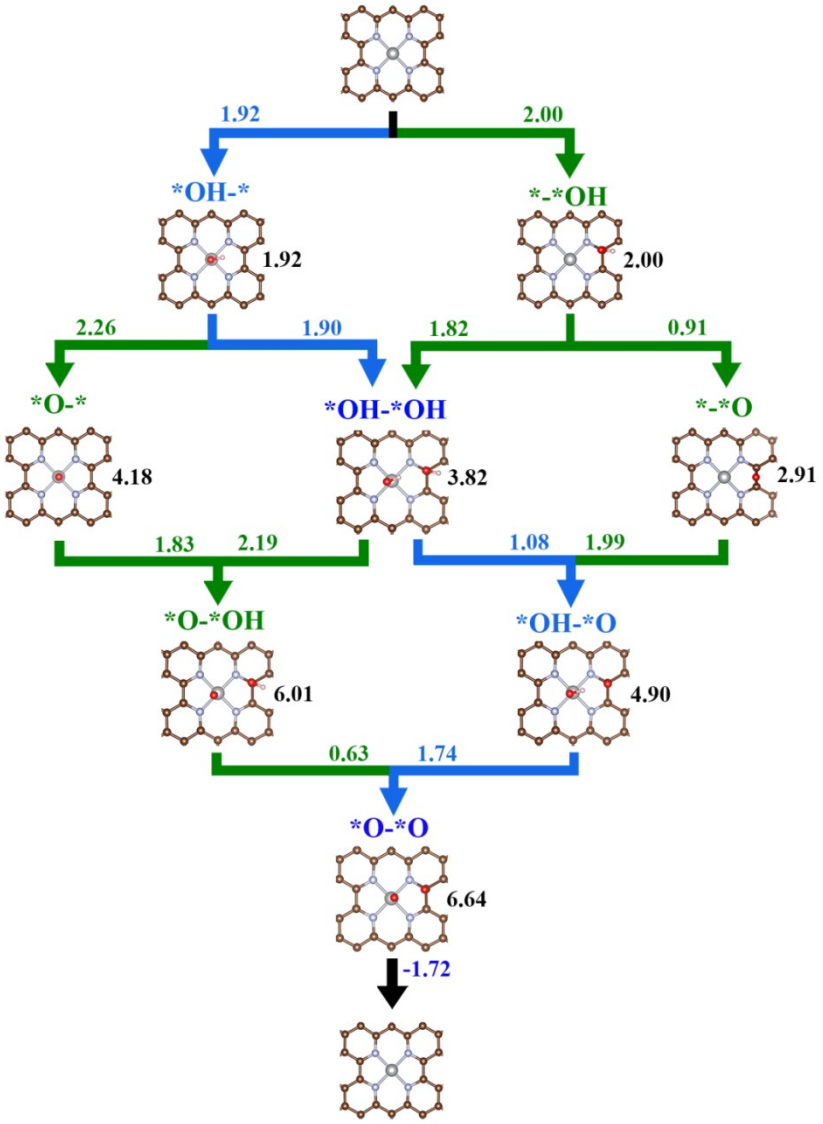


Fig. S14 Calculated free energy changes (eV) for dual-site *O-*O coupling mechanism on NiN_4-gra. Adsorption free energies of corresponding intermediates are given in black. Blue arrows represent the energetically most favorable path.

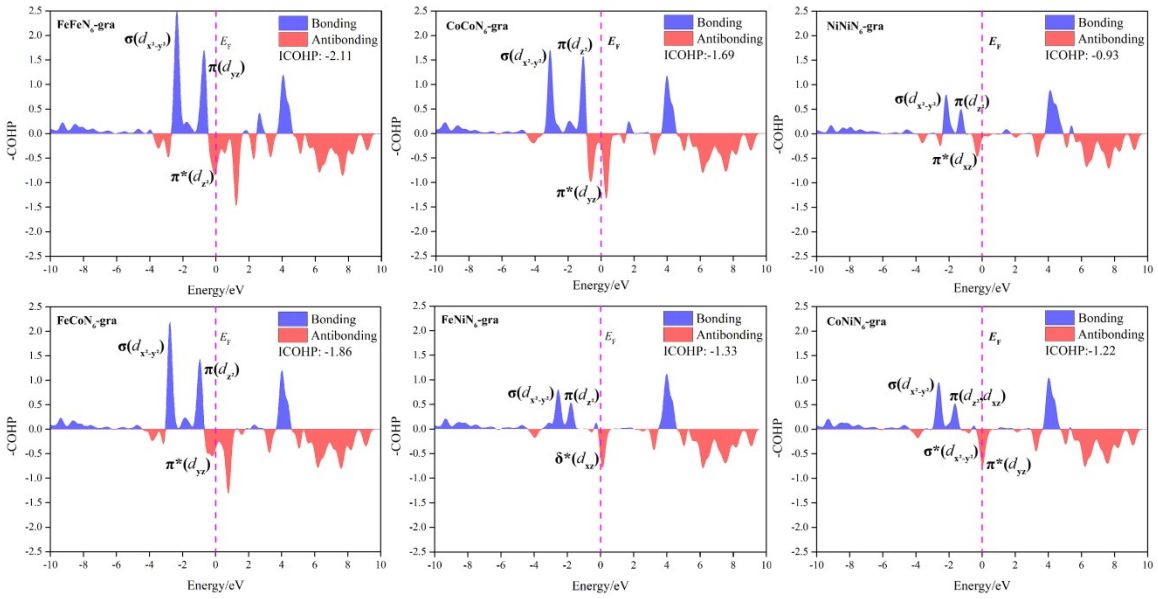
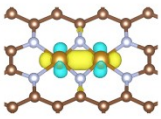
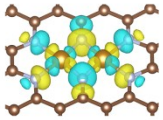
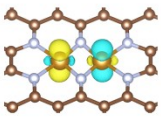
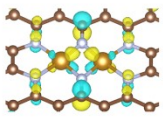
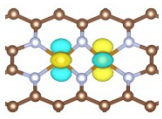
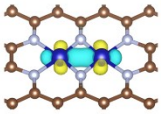
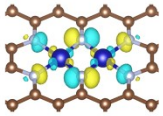
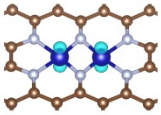
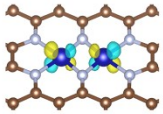
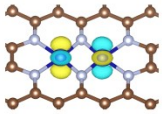
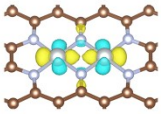
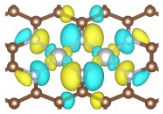
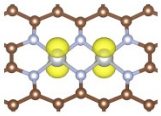
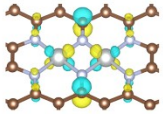
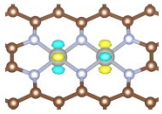
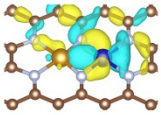
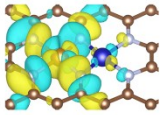
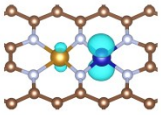
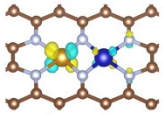
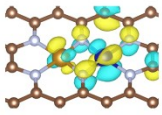
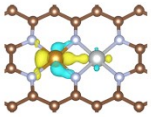
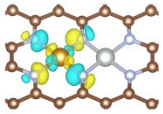
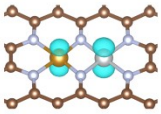
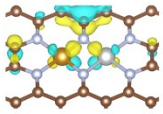
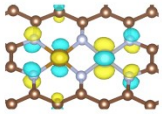
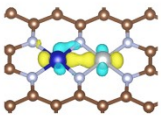
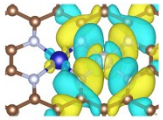
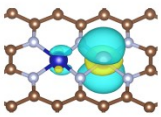
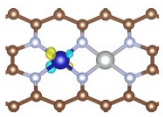
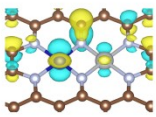


Fig. S15 Crystal orbital Hamilton population (COHP) and integrated-COHP (ICOHP) between the two adjacent metal atoms of MMN_6-gra and $M1M2N_6$-gra.

Table S7 Crystal orbital overlaps between the two adjacent metal atoms of MMN_6-gra and $M1M2N_6$-gra. The isovalues are given in a.u.

Model	d_{x2-y2}	d_{xy}	d_{z2}	d_{yz}	d_{xz}
$FeFeN_6$-gra	 5.0×10^{-7}	 5.0×10^{-8}	 5.0×10^{-7}	 5.0×10^{-8}	 5.0×10^{-7}
$CoCoN_6$-gra	 5.0×10^{-7}	 5.0×10^{-7}	 5.0×10^{-7}	 5.0×10^{-7}	 5.0×10^{-8}
$NiNiN_6$-gra	 5.0×10^{-7}	 2.0×10^{-7}	 5.0×10^{-7}	 2.0×10^{-7}	 5.0×10^{-7}
$FeCoN_6$-gra	 5.0×10^{-7}	 2.0×10^{-7}	 5.0×10^{-7}	 5.0×10^{-7}	 2.0×10^{-7}
$FeNiN_6$-gra	 5.0×10^{-7}	 1.0×10^{-8}	 5.0×10^{-7}	 2.0×10^{-7}	 2.0×10^{-7}
$CoNiN_6$-gra	 5.0×10^{-7}	 1.0×10^{-7}	 5.0×10^{-7}	 5.0×10^{-7}	 2.0×10^{-7}

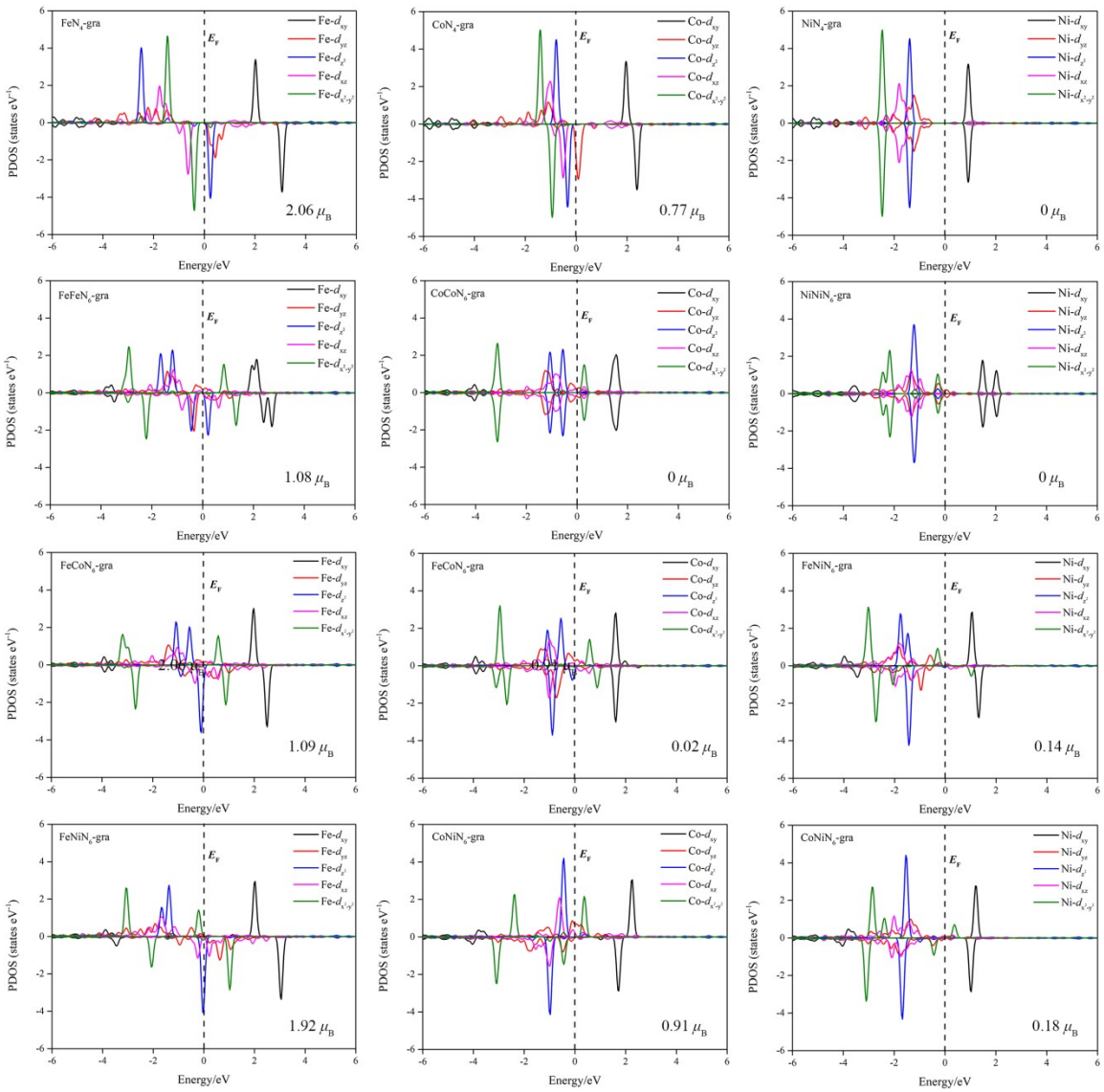


Fig. S16 Projected DOSs of M-3*d* states (both spin up and spin down) and metal spin moment of all catalysts. Fermi levels are set at 0 eV.

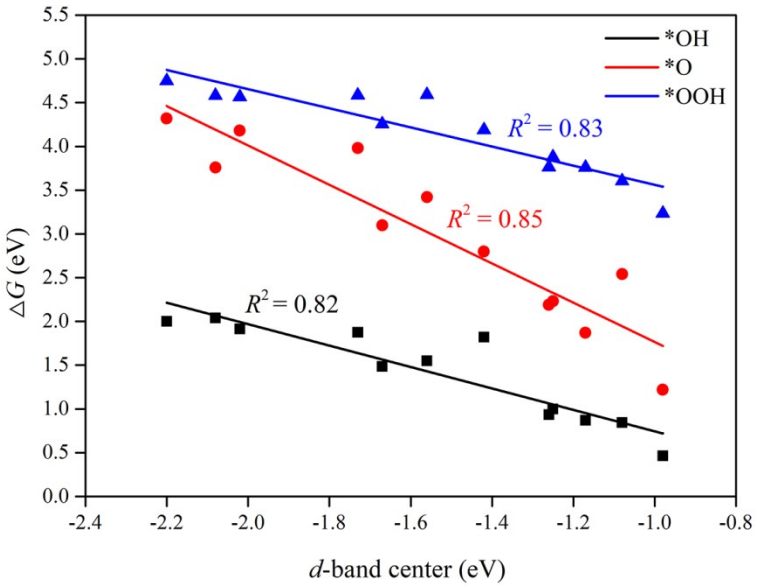


Fig. S17 Linear relationships between the adsorption behaviors and the d-band centers of the metals of all the investigated catalysts.

Table S8 Optimized adsorption structures (distance unit: Å) and adsorption free energies of reaction intermediates involved in single-site OER mechanism on different active sites of $FeFeN_6$-gra.

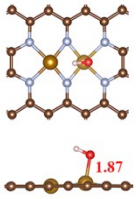
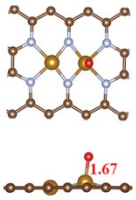
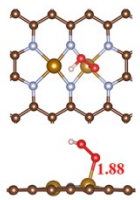
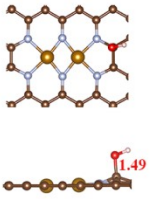
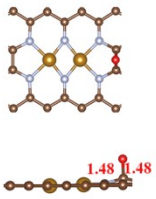
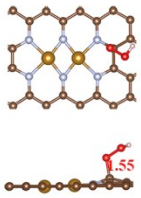
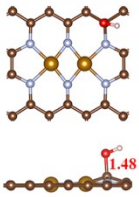
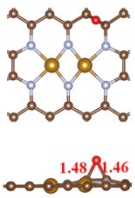
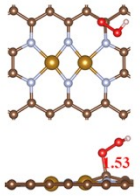
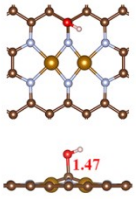
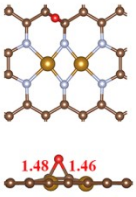
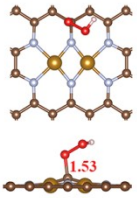
$FeFeN_6$-gra	*OH	*O	*OOH
Fe site	 0.94 eV	 2.19 eV	 3.77 eV
C1 site	 1.47 eV	 2.89 eV	 4.91 eV
C2 site	 1.96 eV	 2.99 eV	 4.99 eV
C3 site	 1.96 eV	 3.27 eV	 5.03 eV

Table S9 Optimized adsorption structures (distance unit: Å) and adsorption free energies of reaction intermediates involved in single-site OER mechanism on different active sites of $CoCoN_6$-gra.

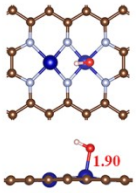
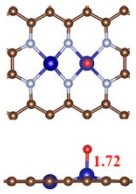
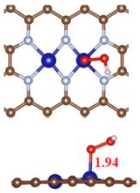
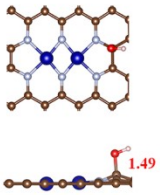
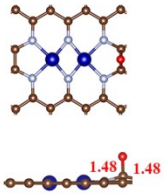
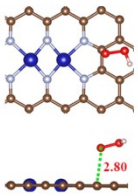
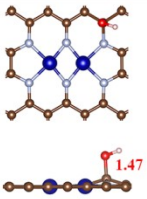
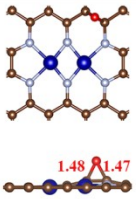
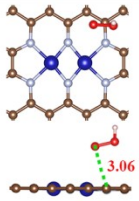
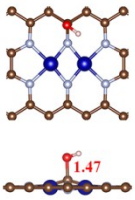
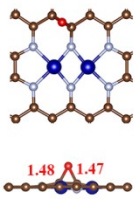
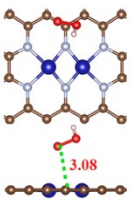
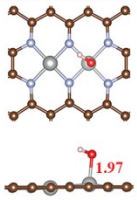
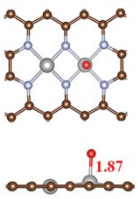
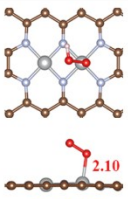
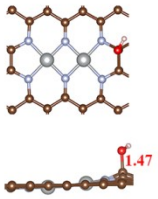
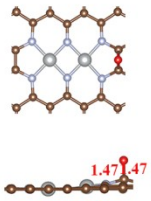
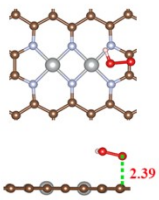
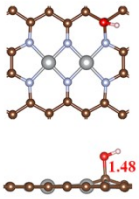
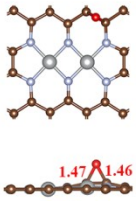
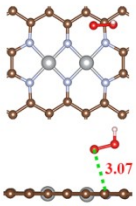
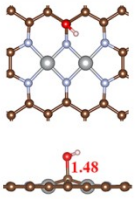
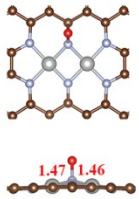
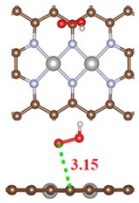
$CoCoN_6$-gra	*OH	*O	*OOH
Co site	 1.49 eV	 3.10 eV	 4.26 eV
C1 site	 1.59 eV	 3.02 eV	 4.96 eV
C2 site	 2.17 eV	 3.10 eV	 4.95 eV
C3 site	 2.12 eV	 3.14 eV	 4.96 eV

Table S10 Optimized adsorption structures (distance unit: Å) and adsorption free energies of reaction intermediates involved in single-site OER mechanism on different active sites of $NiNiN_6$-gra.

$NiNiN_6$-gra	*OH	*O	*OOH
Ni site	 1.88 eV	 4.02 eV	 4.59 eV
C1 site	 1.57 eV	 2.99 eV	 5.02 eV
C2 site	 2.26 eV	 3.02 eV	 4.99 eV
C3 site	 2.43 eV	 3.04 eV	 5.31 eV

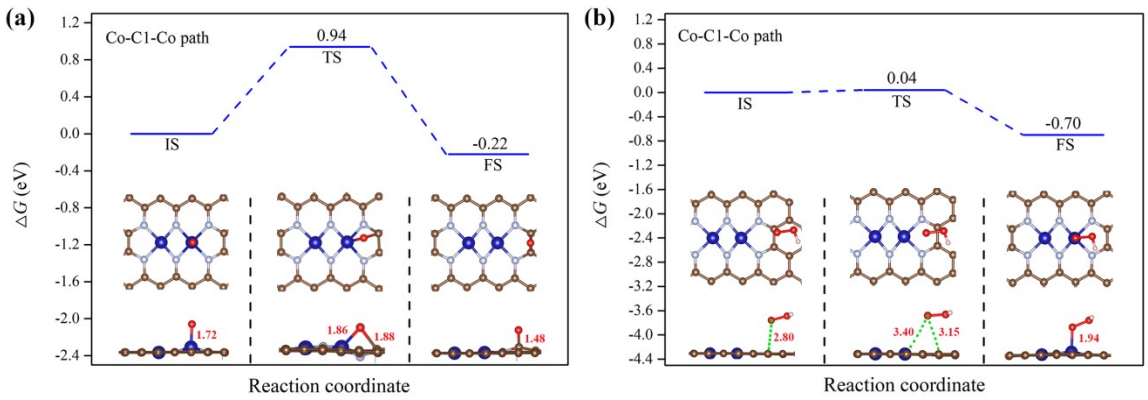


Fig. S18 Calculated free energy barriers for (a) O transfers from the Co to C1 site; (b) OOH transfers from the C1 to Co site of $CoCoN_6$-gra using the NEB method. IS, TS, and FS denote the initial state, transition state and final state, respectively.

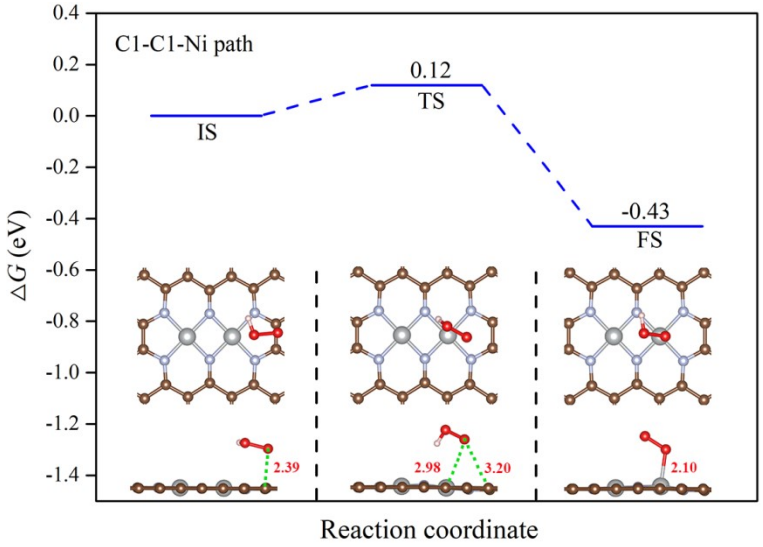


Fig. S19 Calculated free energy barrier for the OOH transfer from the C1 to Ni site of $NiNiN_6$-gra using the NEB method. IS, TS, and FS denote the initial state, transition state and final state, respectively.

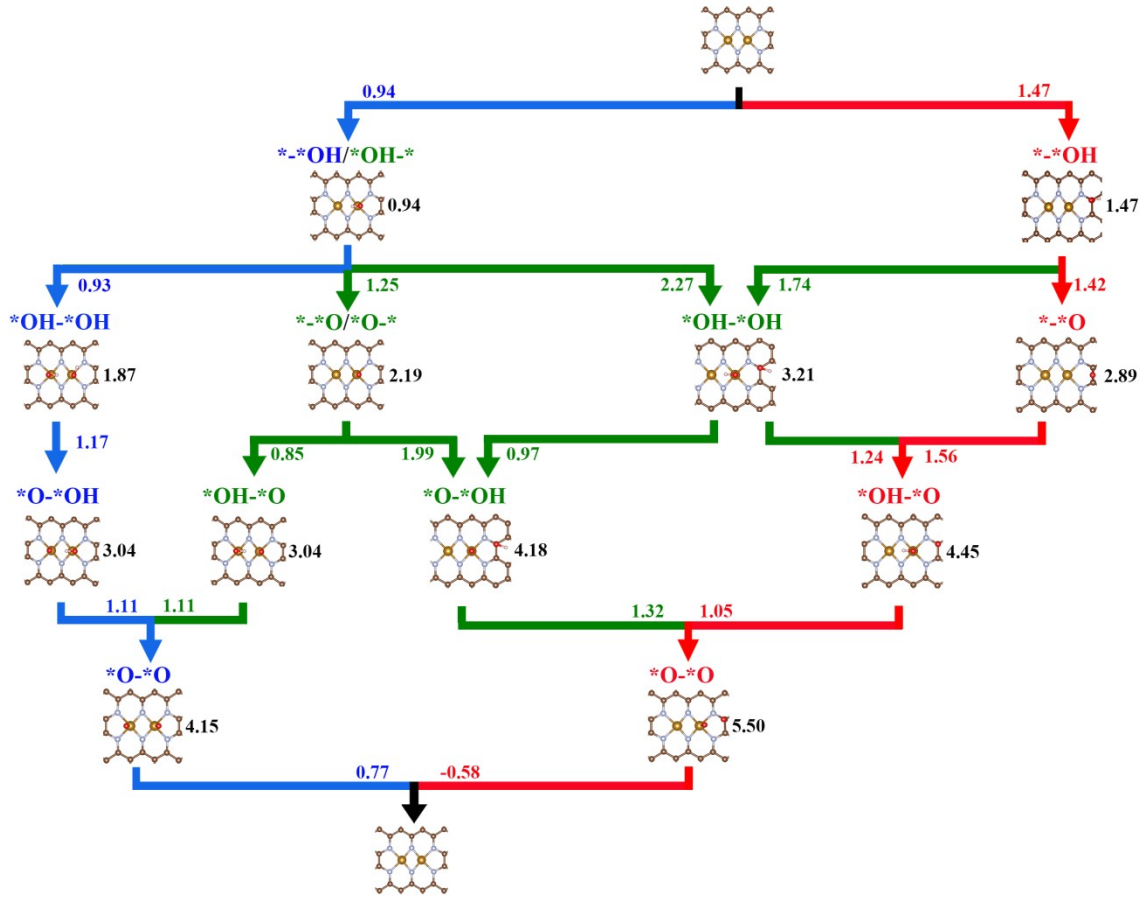


Fig. S20 Calculated free energy changes (eV) for dual-site *O-*O coupling mechanism on $FeFeN_6$-gra. Adsorption free energies of corresponding intermediates are given in black. Blue and red arrows represent the energetically most favorable path for M-M and M-C pathways, respectively.

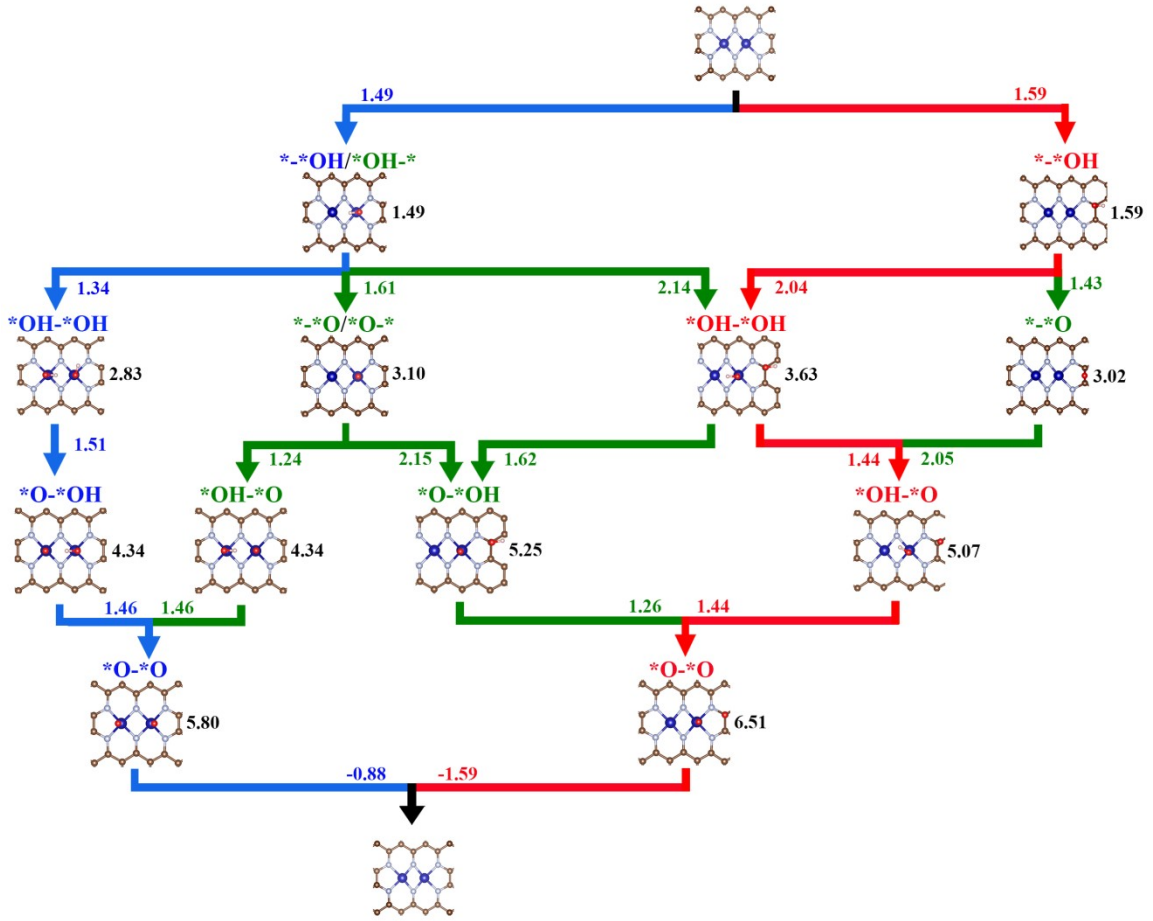


Fig. S21 Calculated free energy changes (eV) for dual-site *O-*O coupling mechanism on $CoCoN_6$-gra. Adsorption free energies of corresponding intermediates are given in black. Blue and red arrows represent the energetically most favorable path for M-M and M-C pathways, respectively.

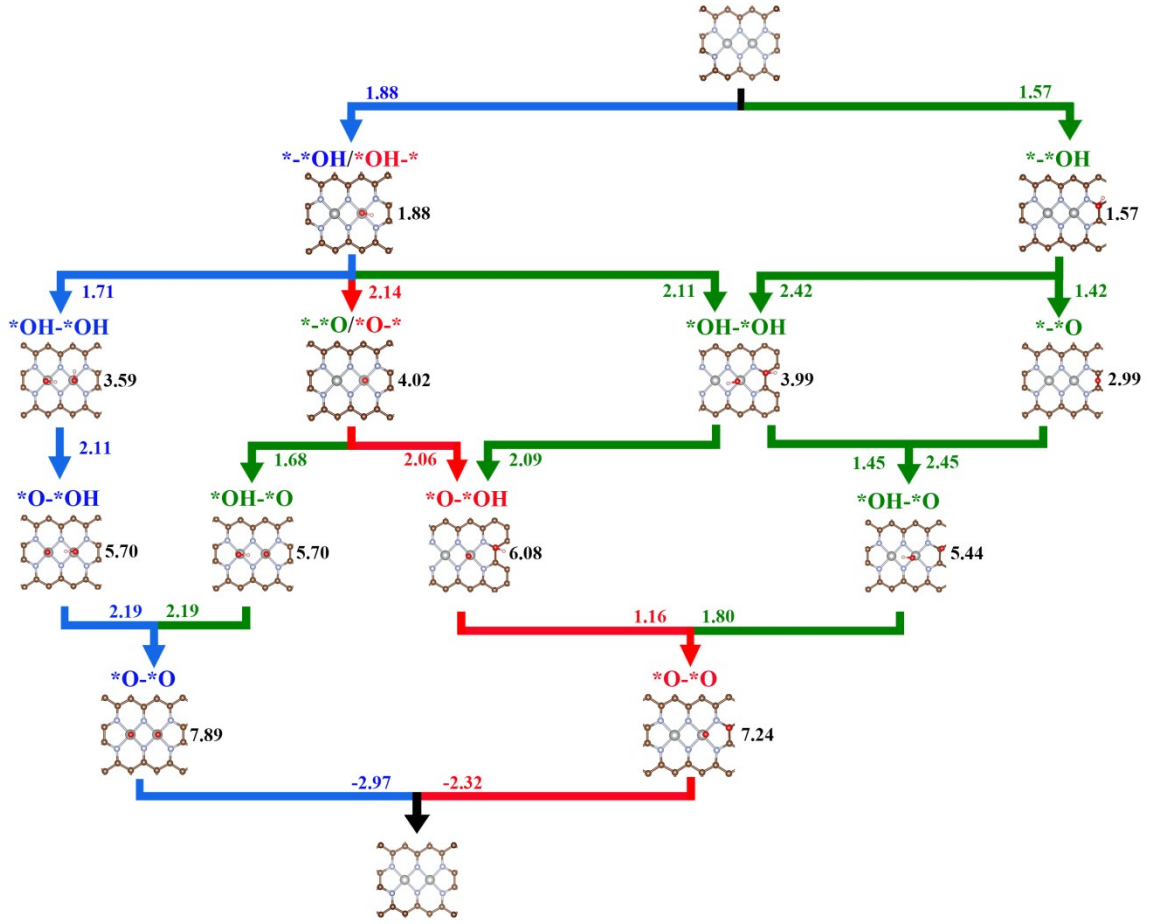


Fig. S22 Calculated free energy changes (eV) for dual-site *O-*O coupling mechanism on $NiNiN_6$-gra. Adsorption free energies of corresponding intermediates are given in black. Blue and red arrows represent the energetically most favorable path for M-M and M-C pathways, respectively.

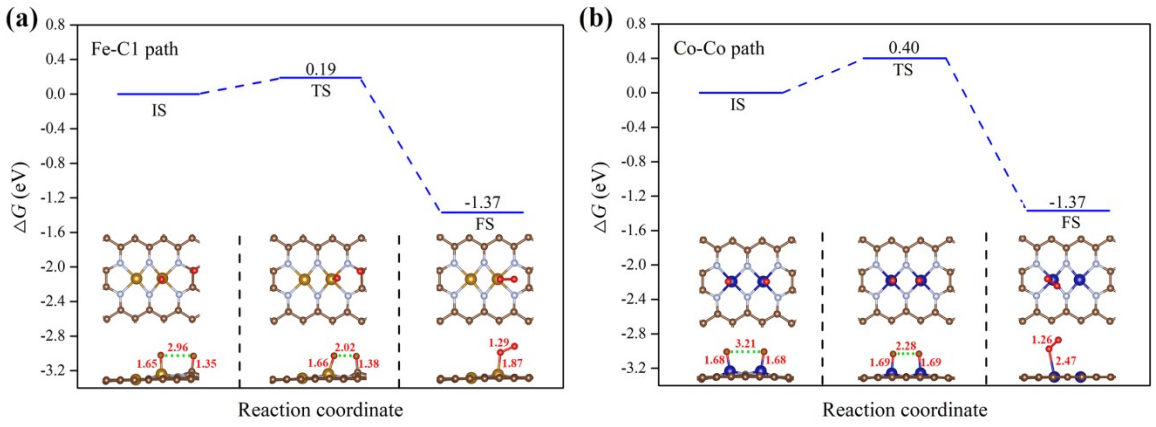


Fig. S23 Calculated free energy profiles for the *O+*O→*O_2 reaction via (a) Fe-C1 path on $FeFeN_6$-gra (b) Co-Co path on $CoCoN_6$-gra. IS, TS, and FS denote the initial state, transition state and final state, respectively.

Table S11 Optimized adsorption structures (distance unit: Å) and adsorption free energies of reaction intermediates involved in single-site OER mechanism on different active sites of $FeCoN_6$-gra.

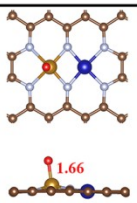
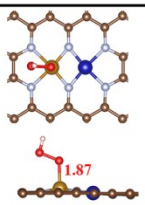
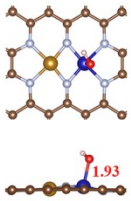
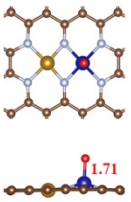
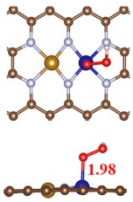
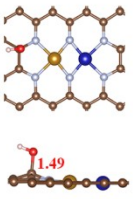
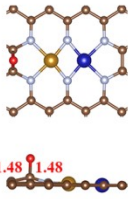
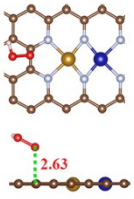
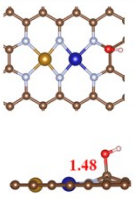
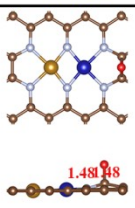
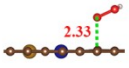
$FeCoN_6$-gra	*OH	*O	*OOH
Fe site	 1.00 eV	 2.23 eV	 3.88 eV
Co site	 1.55 eV	 3.42 eV	 4.59 eV
C_{Fe} site	 1.90 eV	 2.90 eV	 4.84 eV
C_{Co} site	 2.00 eV	 3.03 eV	 5.00 eV

Table S12 Optimized adsorption structures (distance unit: Å) and adsorption free energies of reaction intermediates involved in single-site OER mechanism on different active sites of $FeNiN_6$-gra.

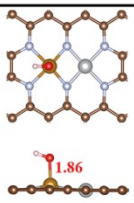
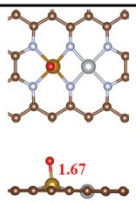
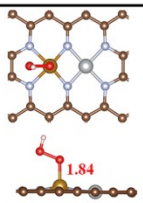
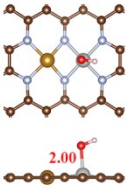
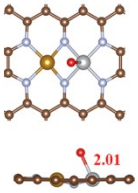
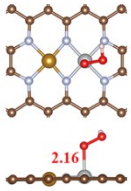
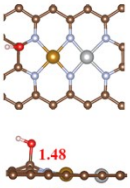
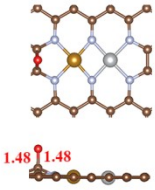
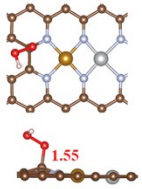
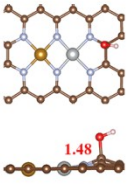
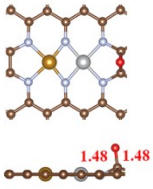
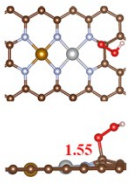
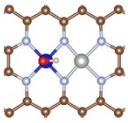
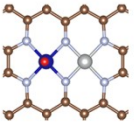
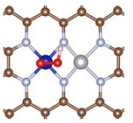
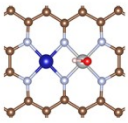
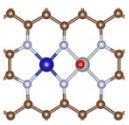
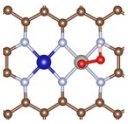
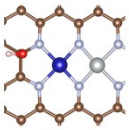
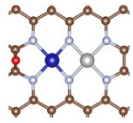
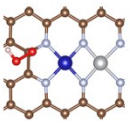
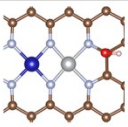
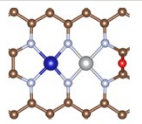
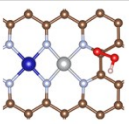
$FeNiN_6$-gra	*OH	*O	*OOH
Fe site	 0.87 eV	 1.87 eV	 3.76 eV
Ni site	 2.04 eV	 3.76 eV	 4.58 eV
C_{Fe} site	 1.76 eV	 2.79 eV	 4.78 eV
C_{Ni} site	 1.83 eV	 3.10 eV	 4.92 eV

Table S13 Optimized adsorption structures (distance unit: Å) and adsorption free energies of reaction intermediates involved in single-site OER mechanism on different active sites of $CoNiN_6$-gra.

$CoNiN_6$-gra	*OH	*O	*OOH
Co site	 1.82 eV	 2.80 eV	 4.19 eV
Ni site	 2.00 eV	 4.32 eV	 4.75 eV
C_{Co} site	 1.90 eV	 2.97 eV	 4.93 eV
C_{Ni} site	 1.90 eV	 3.01 eV	 4.81 eV

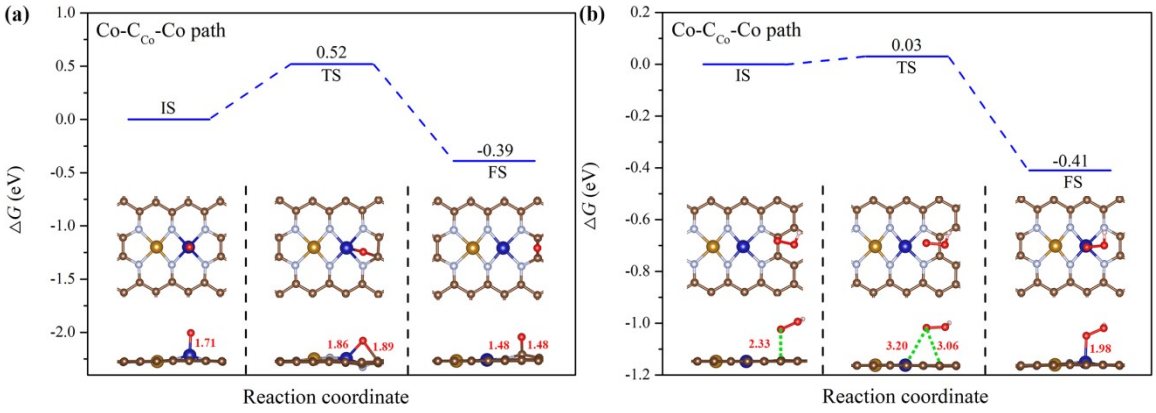


Fig. S24 Calculated free energy barriers for (a) O transfers from the Co to C_{Co} site; (b) OOH transfers from the C_{Co} to Co site of $FeCoN_6$-gra using the NEB method. IS, TS, and FS denote the initial state, transition state and final state, respectively.

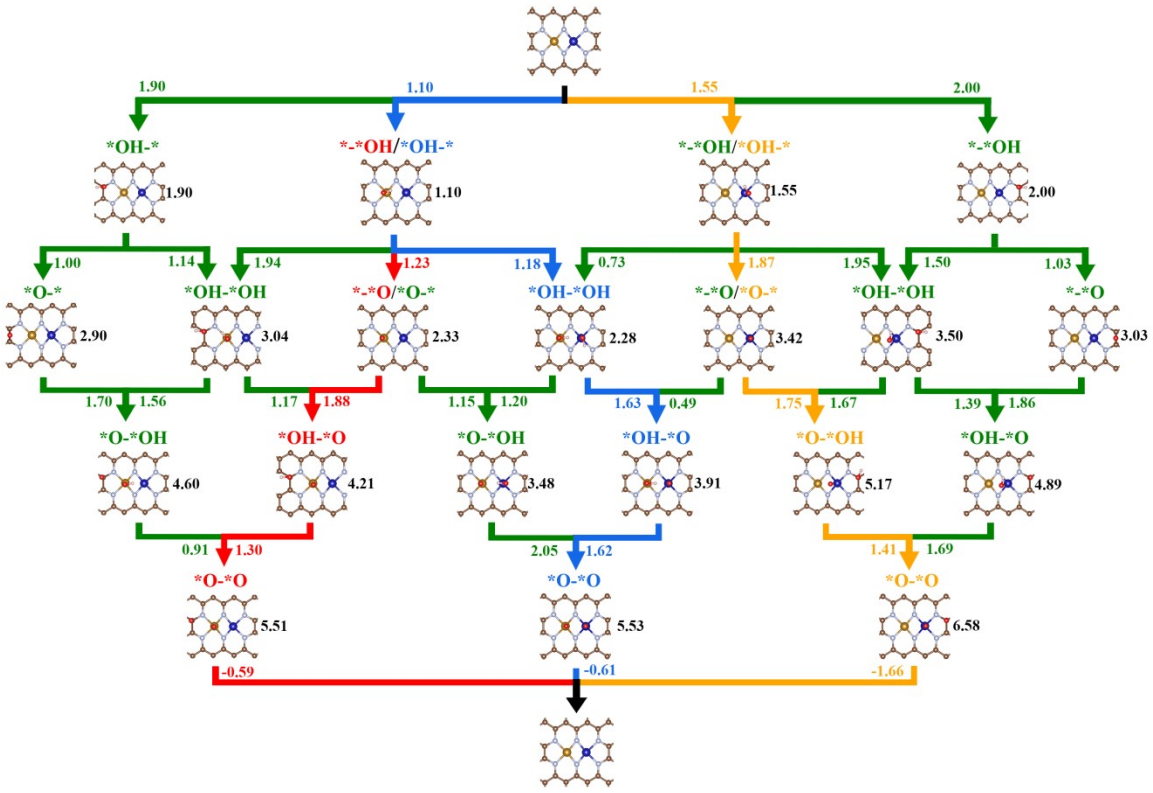


Fig. S25 Calculated free energy changes (eV) for dual-site *O-*O coupling mechanism on $FeCoN_6$-gra. Adsorption free energies of corresponding intermediates are given in black. Blue, red and orange arrows represent the energetically most favorable path for M1-M2, M1-C_{M1} and M2-C_{M2} pathways, respectively.

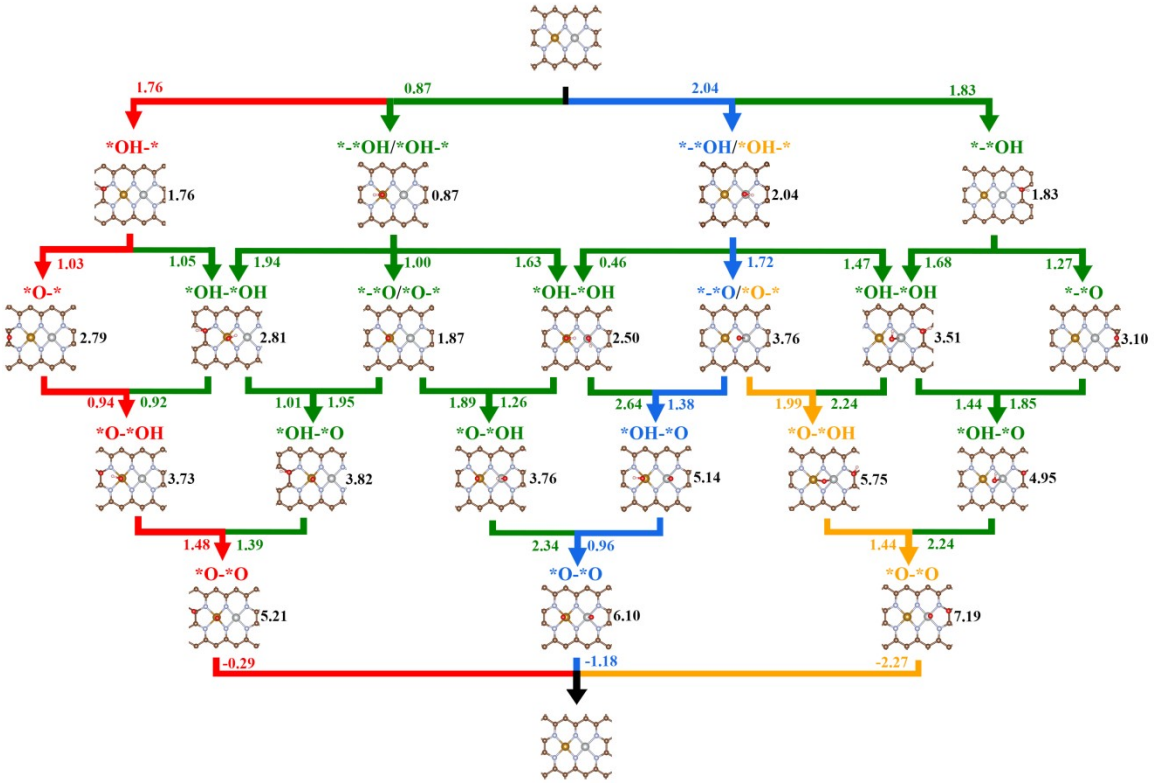


Fig. S26 Calculated free energy changes (eV) for dual-site *O-*O coupling mechanism on $FeNiN_6$-gra. Adsorption free energies of corresponding intermediates are given in black. Blue, red and orange arrows represent the energetically most favorable path for M1-M2, M1-C_{M1} and M2-C_{M2} pathways, respectively.

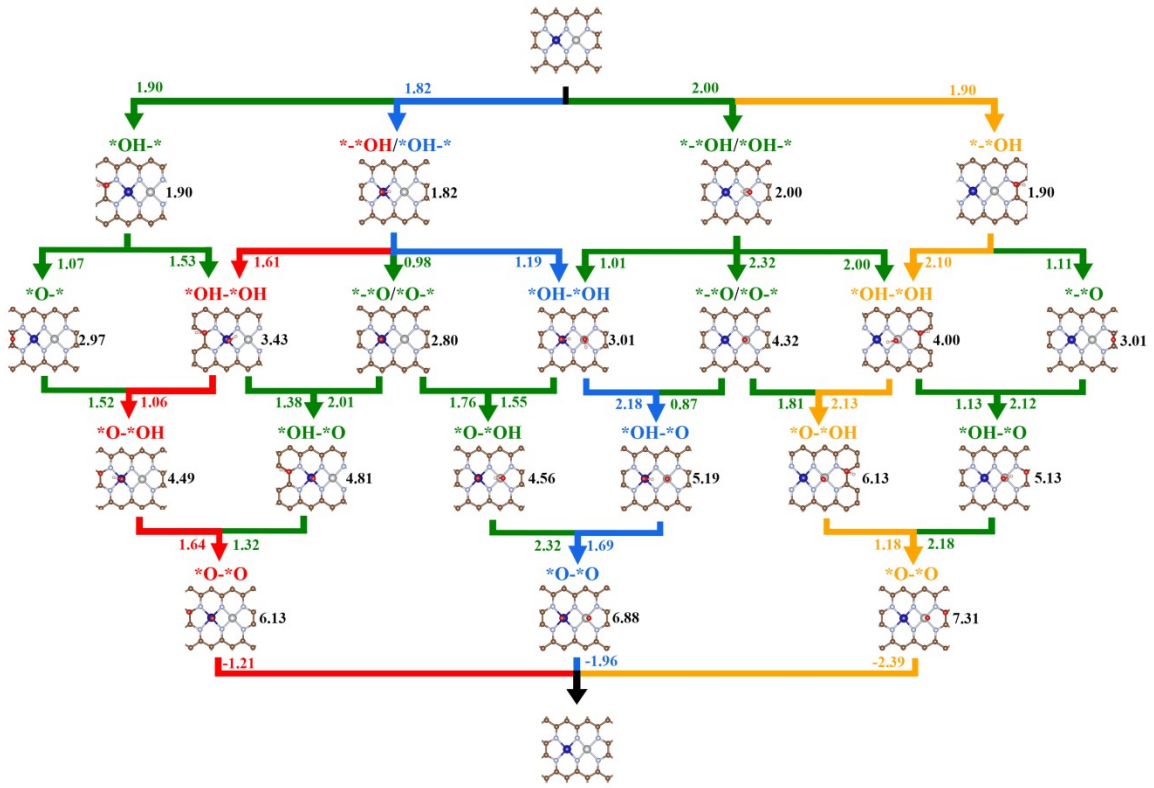


Fig. S27 Calculated free energy changes (eV) for dual-site *O-*O coupling mechanism on $CoNiN_6$-gra. Adsorption free energies of corresponding intermediates are given in black. Blue, red and orange arrows represent the energetically most favorable path for M1-M2, M1-C_{M1} and M2-C_{M2} pathways, respectively.

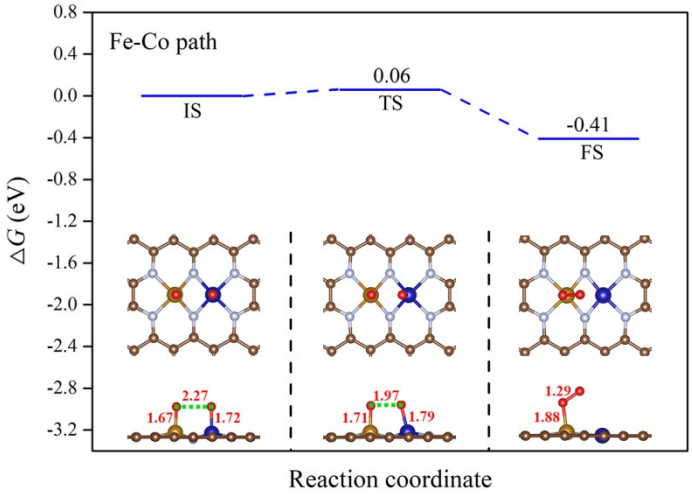


Fig. S28 Calculated free energy profiles for the *O+*O→*O_2 reaction via Fe-Co path on $FeCoN_6$-gra. IS, TS, and FS denote the initial state, transition state and final state, respectively.

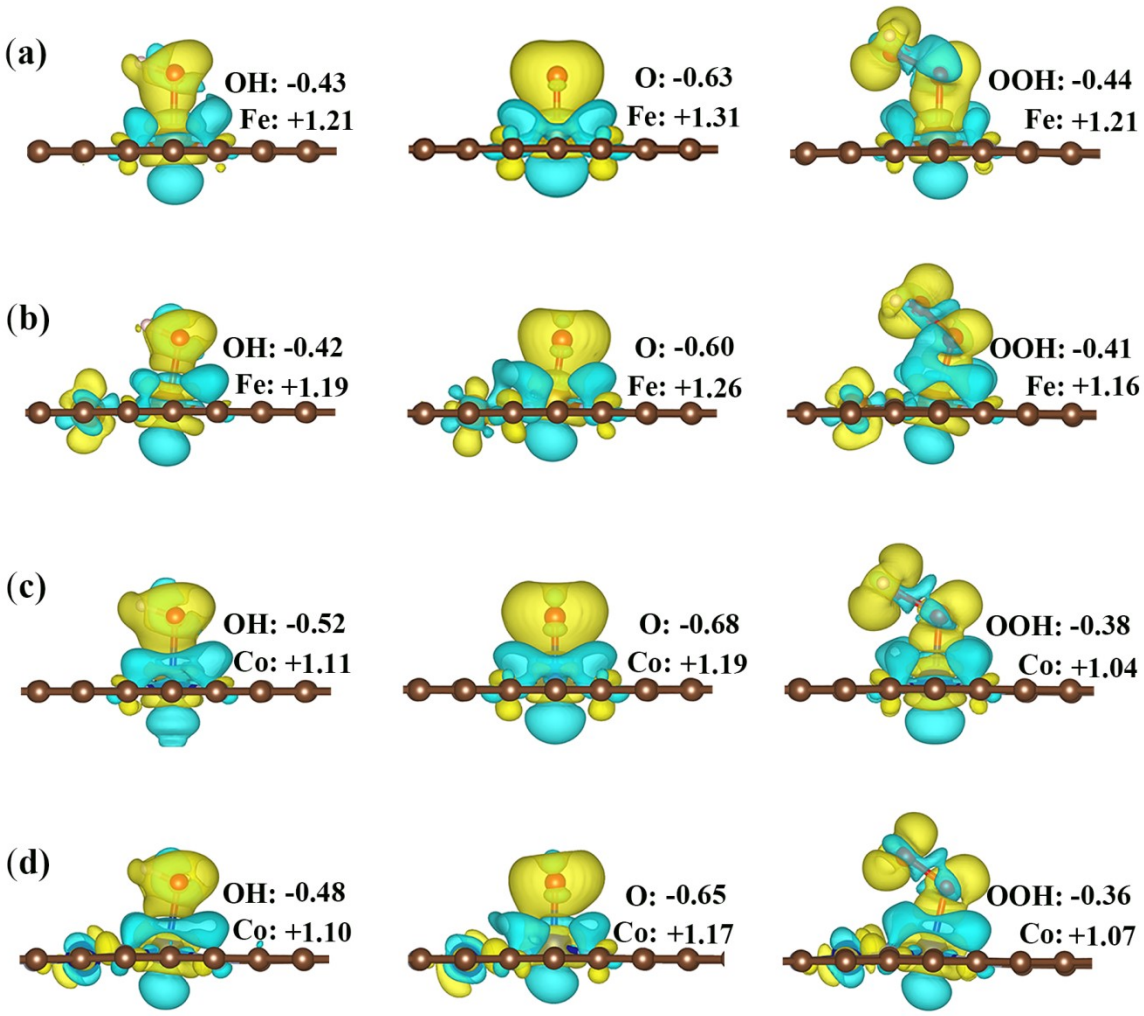


Fig. S29 Charge density difference and Bader charge values during the oxygen evolution reaction. (a) FeN_4-gra, (b) $FeFeN_6$-gra, (c) CoN_4-gra and (d) $CoCoN_6$-gra. For the DACs, only the charge of the metal atom bound to the O-containing species is given.

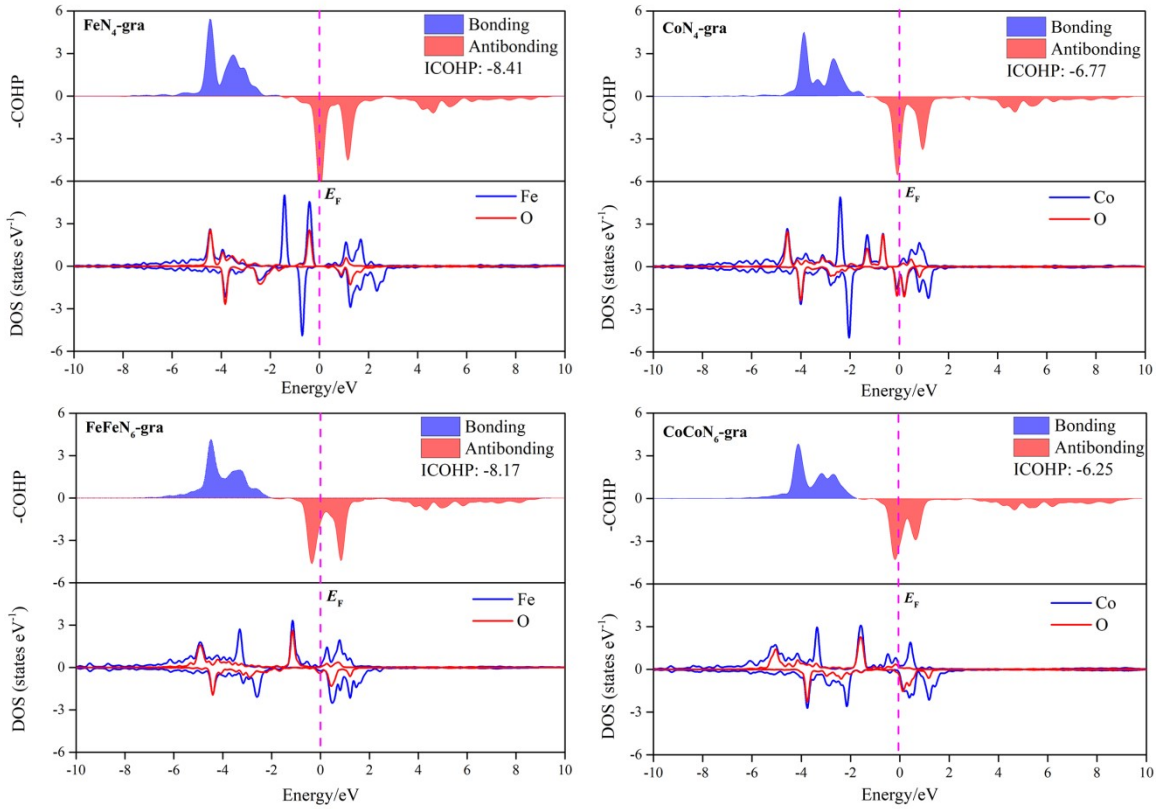


Fig. S30 Crystal orbital Hamiltonian population (COHP) between M-O in *O for FeN_4-gra, CoN_4-gra, $FeFeN_6$-gra and $CoCoN_6$-gra.

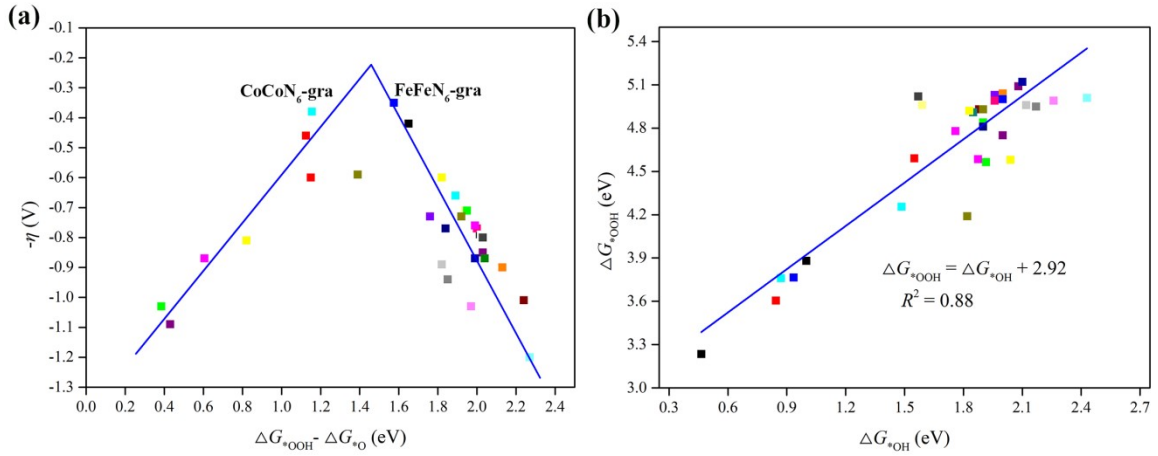


Fig. S31 (a) Volcano-like relationships between single-site OER overpotentials and the ΔG_{*OOH}-ΔG_{*O} descriptor values for all the single atomic sites (both metal and nonmetal atoms) in all the investigated catalysts. (b) linear scaling relationships for the adsorption free energies of different intermediates on all single atomic sites.

CIF files of all the studied catalysts.

FeN_4-gra

```
#======================================================================


# CRYSTAL DATA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CoN_4-gra

#==

CRYSTAL DATA

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C85	1.0	0.523257	0.918566	0.000000	Biso	1.000000	C
C86	1.0	0.570065	0.869426	0.000000	Biso	1.000000	C
C87	1.0	0.665150	0.915905	-0.000000	Biso	1.000000	C
C88	1.0	0.712005	0.867021	0.000000	Biso	1.000000	C
C89	1.0	0.807234	0.915210	0.000000	Biso	1.000000	C
C90	1.0	0.854305	0.867059	0.000000	Biso	1.000000	C
C91	1.0	0.950054	0.915958	-0.000000	Biso	1.000000	C

C92 1.0 0.998654 0.869471 0.000000 Biso 1.000000 C

N1 1.0 0.426088 0.304275 -0.000003 Biso 1.000000 N

N2 1.0 0.577625 0.304306 -0.000003 Biso 1.000000 N

N3 1.0 0.515736 0.483658 -0.000004 Biso 1.000000 N

N4 1.0 0.667248 0.483657 -0.000004 Biso 1.000000 N

Co1 1.0 0.546646 0.394014 -0.000007 Biso 1.000000 Co

NiN_4-gra

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CRYSTAL DATA

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data_VESTA_phase_1

_chemical_name_common 'TM '

_cell_length_a 17.22000

_cell_length_b 17.22000

_cell_length_c 15.00000

_cell_angle_alpha 90

_cell_angle_beta 90

_cell_angle_gamma 120

_space_group_name_H-M_alt 'P 1'

_space_group_IT_number 1

loop_

_space_group_symop_operation_xyz

'x, y, z'

loop_

_atom_site_label

_atom_site_occupancy

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

_atom_site_adp_type

_atom_site_B_iso_or_equiv

_atom_site_type_symbol

C1	1.0	0.093636	0.060312	0.000000	Biso	1.000000	C
C2	1.0	0.142747	0.014350	0.000000	Biso	1.000000	C
C3	1.0	0.238854	0.063666	-0.000000	Biso	1.000000	C
C4	1.0	0.287297	0.016990	-0.000000	Biso	1.000000	C
C5	1.0	0.383129	0.066818	-0.000001	Biso	1.000000	C
C6	1.0	0.429087	0.016977	-0.000000	Biso	1.000000	C
C7	1.0	0.524206	0.063667	-0.000001	Biso	1.000000	C
C8	1.0	0.570941	0.014333	0.000000	Biso	1.000000	C
C9	1.0	0.666000	0.060307	0.000000	Biso	1.000000	C
C10	1.0	0.712886	0.011636	-0.000000	Biso	1.000000	C
C11	1.0	0.808032	0.059141	-0.000000	Biso	1.000000	C
C12	1.0	0.855132	0.011016	-0.000000	Biso	1.000000	C
C13	1.0	0.950371	0.059152	-0.000000	Biso	1.000000	C
C14	1.0	0.998043	0.011673	-0.000000	Biso	1.000000	C
C15	1.0	0.093048	0.202891	0.000000	Biso	1.000000	C
C16	1.0	0.140898	0.155594	0.000001	Biso	1.000000	C
C17	1.0	0.235978	0.204090	-0.000000	Biso	1.000000	C
C18	1.0	0.286423	0.159569	-0.000001	Biso	1.000000	C
C19	1.0	0.382992	0.211482	-0.000002	Biso	1.000000	C
C20	1.0	0.431779	0.164078	-0.000003	Biso	1.000000	C
C21	1.0	0.527967	0.211505	-0.000002	Biso	1.000000	C
C22	1.0	0.572585	0.159584	-0.000001	Biso	1.000000	C
C23	1.0	0.667542	0.204127	-0.000000	Biso	1.000000	C
C24	1.0	0.714059	0.155597	0.000001	Biso	1.000000	C
C25	1.0	0.809192	0.202918	0.000000	Biso	1.000000	C

C26	1.0	0.855960	0.154749	-0.000000	Biso	1.000000	C
C27	1.0	0.950985	0.202687	-0.000000	Biso	1.000000	C
C28	1.0	0.998082	0.154753	-0.000000	Biso	1.000000	C
C29	1.0	0.093511	0.346271	0.000000	Biso	1.000000	C
C30	1.0	0.140328	0.298270	0.000001	Biso	1.000000	C
C31	1.0	0.234972	0.346568	0.000001	Biso	1.000000	C
C32	1.0	0.282325	0.299075	-0.000001	Biso	1.000000	C
C33	1.0	0.376289	0.346399	-0.000002	Biso	1.000000	C
C34	1.0	0.669553	0.346434	-0.000002	Biso	1.000000	C
C35	1.0	0.716191	0.299118	-0.000001	Biso	1.000000	C
C36	1.0	0.811019	0.346641	0.000001	Biso	1.000000	C
C37	1.0	0.857307	0.298306	0.000001	Biso	1.000000	C
C38	1.0	0.952109	0.346318	0.000000	Biso	1.000000	C
C39	1.0	0.998718	0.298127	-0.000000	Biso	1.000000	C
C40	1.0	0.094653	0.489994	-0.000000	Biso	1.000000	C
C41	1.0	0.141278	0.441809	0.000000	Biso	1.000000	C
C42	1.0	0.236077	0.489764	0.000001	Biso	1.000000	C
C43	1.0	0.282374	0.441404	0.000001	Biso	1.000000	C
C44	1.0	0.377202	0.488882	-0.000001	Biso	1.000000	C
C45	1.0	0.423830	0.441533	-0.000003	Biso	1.000000	C
C46	1.0	0.717086	0.441559	-0.000003	Biso	1.000000	C
C47	1.0	0.811052	0.488930	-0.000001	Biso	1.000000	C
C48	1.0	0.858418	0.441475	0.000001	Biso	1.000000	C
C49	1.0	0.953047	0.489836	0.000001	Biso	1.000000	C
C50	1.0	0.999863	0.441851	0.000000	Biso	1.000000	C
C51	1.0	0.095245	0.633343	-0.000000	Biso	1.000000	C
C52	1.0	0.142357	0.585424	-0.000000	Biso	1.000000	C
C53	1.0	0.237377	0.633321	-0.000000	Biso	1.000000	C
C54	1.0	0.284167	0.585150	0.000000	Biso	1.000000	C
C55	1.0	0.379292	0.632424	0.000000	Biso	1.000000	C
C56	1.0	0.425817	0.583876	-0.000001	Biso	1.000000	C
C57	1.0	0.520756	0.628365	-0.000002	Biso	1.000000	C

C58	1.0	0.565395	0.576446	-0.000003	Biso	1.000000	C
C59	1.0	0.661585	0.623856	-0.000003	Biso	1.000000	C
C60	1.0	0.710348	0.576440	-0.000003	Biso	1.000000	C
C61	1.0	0.806907	0.628395	-0.000002	Biso	1.000000	C
C62	1.0	0.857364	0.583913	-0.000001	Biso	1.000000	C
C63	1.0	0.952438	0.632479	0.000001	Biso	1.000000	C
C64	1.0	0.000295	0.585210	0.000001	Biso	1.000000	C
C65	1.0	0.095242	0.776395	-0.000000	Biso	1.000000	C
C66	1.0	0.142923	0.728922	-0.000000	Biso	1.000000	C
C67	1.0	0.238149	0.777007	-0.000000	Biso	1.000000	C
C68	1.0	0.285272	0.728903	-0.000000	Biso	1.000000	C
C69	1.0	0.380422	0.776372	-0.000000	Biso	1.000000	C
C70	1.0	0.427330	0.727704	0.000000	Biso	1.000000	C
C71	1.0	0.522384	0.773648	0.000000	Biso	1.000000	C
C72	1.0	0.569111	0.724280	-0.000001	Biso	1.000000	C
C73	1.0	0.664226	0.770954	-0.000000	Biso	1.000000	C
C74	1.0	0.710210	0.721126	-0.000001	Biso	1.000000	C
C75	1.0	0.806025	0.770992	-0.000000	Biso	1.000000	C
C76	1.0	0.854449	0.724313	-0.000001	Biso	1.000000	C
C77	1.0	0.950545	0.773696	0.000000	Biso	1.000000	C
C78	1.0	0.999657	0.727756	0.000000	Biso	1.000000	C
C79	1.0	0.094624	0.918585	0.000000	Biso	1.000000	C
C80	1.0	0.143214	0.872076	0.000000	Biso	1.000000	C
C81	1.0	0.238962	0.920886	0.000000	Biso	1.000000	C
C82	1.0	0.286030	0.872741	0.000000	Biso	1.000000	C
C83	1.0	0.381252	0.920868	0.000000	Biso	1.000000	C
C84	1.0	0.428166	0.872054	-0.000000	Biso	1.000000	C
C85	1.0	0.523258	0.918560	0.000000	Biso	1.000000	C
C86	1.0	0.570059	0.869427	0.000000	Biso	1.000000	C
C87	1.0	0.665149	0.915932	0.000000	Biso	1.000000	C
C88	1.0	0.712035	0.867078	0.000000	Biso	1.000000	C
C89	1.0	0.807255	0.915256	0.000000	Biso	1.000000	C

C90 1.0 0.854329 0.867116 0.000000 Biso 1.000000 C

C91 1.0 0.950075 0.915981 -0.000000 Biso 1.000000 C

C92 1.0 0.998659 0.869475 0.000000 Biso 1.000000 C

N1 1.0 0.425924 0.304053 -0.000003 Biso 1.000000 N

N2 1.0 0.577584 0.304084 -0.000003 Biso 1.000000 N

N3 1.0 0.515789 0.483881 -0.000003 Biso 1.000000 N

N4 1.0 0.667428 0.483880 -0.000003 Biso 1.000000 N

Ni1 1.0 0.546653 0.393992 -0.000006 Biso 1.000000 Ni

$FeFeN_6$-gra

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CRYSTAL DATA

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data_VESTA_phase_1

_chemical_name_common 'TM2 '

_cell_length_a 17.22000

_cell_length_b 17.22000

_cell_length_c 15.03910

_cell_angle_alpha 90

_cell_angle_beta 90

_cell_angle_gamma 120

_space_group_name_H-M_alt 'P 1'

_space_group_IT_number 1

loop_

_space_group_symop_operation_xyz

'x, y, z'

loop_

_atom_site_label

_atom_site_occupancy

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

_atom_site_adp_type

_atom_site_B_iso_or_equiv

_atom_site_type_symbol

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C3	1.0	0.144065	0.129992	0.000011	Biso	1.000000	C
C4	1.0	0.192263	0.083160	0.999986	Biso	1.000000	C
C5	1.0	0.288190	0.133316	0.000024	Biso	1.000000	C
C6	1.0	0.335867	0.085189	0.999980	Biso	1.000000	C
C7	1.0	0.431684	0.133304	0.000020	Biso	1.000000	C
C8	1.0	0.477467	0.083160	0.999960	Biso	1.000000	C
C9	1.0	0.572487	0.129979	0.999967	Biso	1.000000	C
C10	1.0	0.619043	0.080463	0.999983	Biso	1.000000	C
C11	1.0	0.714111	0.126772	0.999988	Biso	1.000000	C
C12	1.0	0.760996	0.078102	0.000010	Biso	1.000000	C
C13	1.0	0.856237	0.125954	0.000015	Biso	1.000000	C
C14	1.0	0.903635	0.078114	0.000007	Biso	1.000000	C
C15	1.0	0.999070	0.269754	0.999993	Biso	1.000000	C
C16	1.0	0.046639	0.222224	0.999985	Biso	1.000000	C
C17	1.0	0.141672	0.270847	0.999999	Biso	1.000000	C
C18	1.0	0.191781	0.226101	0.000038	Biso	1.000000	C
C19	1.0	0.288066	0.277974	0.000100	Biso	1.000000	C
C20	1.0	0.335973	0.229947	0.000129	Biso	1.000000	C
C21	1.0	0.432411	0.278260	0.000303	Biso	1.000000	C
C22	1.0	0.480514	0.229931	0.000191	Biso	1.000000	C
C23	1.0	0.576438	0.277950	0.000138	Biso	1.000000	C

C24	1.0	0.620862	0.226082	0.999987	Biso	1.000000	C
C25	1.0	0.715691	0.270832	0.999976	Biso	1.000000	C
C26	1.0	0.762101	0.222214	0.999969	Biso	1.000000	C
C27	1.0	0.857186	0.269745	0.999986	Biso	1.000000	C
C28	1.0	0.904077	0.221640	0.000010	Biso	1.000000	C
C29	1.0	0.999860	0.413270	0.999987	Biso	1.000000	C
C30	1.0	0.046544	0.365155	0.999986	Biso	1.000000	C
C31	1.0	0.141219	0.413596	0.999973	Biso	1.000000	C
C32	1.0	0.188489	0.365987	0.999991	Biso	1.000000	C
C33	1.0	0.282527	0.413468	0.000011	Biso	1.000000	C
C34	1.0	0.717359	0.413432	0.000149	Biso	1.000000	C
C35	1.0	0.763935	0.365964	0.999996	Biso	1.000000	C
C36	1.0	0.858801	0.413572	0.999941	Biso	1.000000	C
C37	1.0	0.905058	0.365143	0.999965	Biso	1.000000	C
C38	1.0	0.000918	0.556909	0.999966	Biso	1.000000	C
C39	1.0	0.047596	0.508775	0.999988	Biso	1.000000	C
C40	1.0	0.142400	0.556929	0.999987	Biso	1.000000	C
C41	1.0	0.188651	0.508507	0.999973	Biso	1.000000	C
C42	1.0	0.283531	0.556168	0.999992	Biso	1.000000	C
C43	1.0	0.330137	0.508733	0.000013	Biso	1.000000	C
C44	1.0	0.764951	0.508700	0.000149	Biso	1.000000	C
C45	1.0	0.858984	0.556136	0.999998	Biso	1.000000	C
C46	1.0	0.906230	0.508488	0.999940	Biso	1.000000	C
C47	1.0	0.000878	0.699879	0.999970	Biso	1.000000	C
C48	1.0	0.048424	0.652326	0.999987	Biso	1.000000	C
C49	1.0	0.143431	0.700461	0.000011	Biso	1.000000	C
C50	1.0	0.190307	0.652344	0.999995	Biso	1.000000	C
C51	1.0	0.285405	0.699918	0.999986	Biso	1.000000	C
C52	1.0	0.331817	0.651316	0.000000	Biso	1.000000	C
C53	1.0	0.426661	0.696114	0.000041	Biso	1.000000	C
C54	1.0	0.471096	0.644289	0.000107	Biso	1.000000	C
C55	1.0	0.567039	0.692340	0.000148	Biso	1.000000	C

C56	1.0	0.615142	0.644009	0.000326	Biso	1.000000	C
C57	1.0	0.711581	0.692301	0.000209	Biso	1.000000	C
C58	1.0	0.759483	0.644257	0.000143	Biso	1.000000	C
C59	1.0	0.855774	0.696082	0.999989	Biso	1.000000	C
C60	1.0	0.905837	0.651283	0.999979	Biso	1.000000	C
C61	1.0	0.999628	0.841665	0.999981	Biso	1.000000	C
C62	1.0	0.048357	0.795332	0.999988	Biso	1.000000	C
C63	1.0	0.143939	0.844028	0.000010	Biso	1.000000	C
C64	1.0	0.191297	0.796163	0.000015	Biso	1.000000	C
C65	1.0	0.286549	0.844049	0.000007	Biso	1.000000	C
C66	1.0	0.333415	0.795372	0.999996	Biso	1.000000	C
C67	1.0	0.428483	0.841691	0.999999	Biso	1.000000	C
C68	1.0	0.475059	0.792210	0.000012	Biso	1.000000	C
C69	1.0	0.570087	0.839062	0.999988	Biso	1.000000	C
C70	1.0	0.615892	0.788964	0.000031	Biso	1.000000	C
C71	1.0	0.711715	0.837073	0.999985	Biso	1.000000	C
C72	1.0	0.759399	0.788941	0.000025	Biso	1.000000	C
C73	1.0	0.855334	0.839036	0.999959	Biso	1.000000	C
C74	1.0	0.903521	0.792188	0.999967	Biso	1.000000	C
C75	1.0	0.999654	0.984444	0.999987	Biso	1.000000	C
C76	1.0	0.047956	0.937692	0.999985	Biso	1.000000	C
C77	1.0	0.143996	0.987061	0.999975	Biso	1.000000	C
C78	1.0	0.192015	0.939893	0.999991	Biso	1.000000	C
C79	1.0	0.287664	0.988786	0.999972	Biso	1.000000	C
C80	1.0	0.334426	0.939922	0.999991	Biso	1.000000	C
C81	1.0	0.429616	0.987073	0.999971	Biso	1.000000	C
C82	1.0	0.476239	0.937702	0.999988	Biso	1.000000	C
C83	1.0	0.571293	0.984457	0.999986	Biso	1.000000	C
C84	1.0	0.617957	0.935133	0.999976	Biso	1.000000	C
C85	1.0	0.713154	0.982270	0.999991	Biso	1.000000	C
C86	1.0	0.759945	0.933438	0.999974	Biso	1.000000	C
C87	1.0	0.855599	0.982273	0.999990	Biso	1.000000	C

C88	1.0	0.903624	0.935112	0.999970	Biso	1.000000 C
N1	1.0	0.332463	0.371258	0.000088	Biso	1.000000 N
N2	1.0	0.477292	0.368115	0.000553	Biso	1.000000 N
N3	1.0	0.625241	0.371226	0.000318	Biso	1.000000 N
N4	1.0	0.422272	0.550996	0.000091	Biso	1.000000 N
N5	1.0	0.570239	0.554170	0.000578	Biso	1.000000 N
N6	1.0	0.715043	0.550962	0.000317	Biso	1.000000 N
Fe1	1.0	0.458501	0.461101	0.000449	Biso	1.000000 Fe
Fe2	1.0	0.589028	0.461175	0.000587	Biso	1.000000 Fe

$CoCoN_6$-gra

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CRYSTAL DATA

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data_VESTA_phase_1

_chemical_name_common 'TM2 '

_cell_length_a 17.22000

_cell_length_b 17.22000

_cell_length_c 15.03910

_cell_angle_alpha 90

_cell_angle_beta 90

_cell_angle_gamma 120

_space_group_name_H-M_alt 'P 1'

_space_group_IT_number 1

loop_

_space_group_symop_operation_xyz

'x, y, z'

loop_

_atom_site_label

_atom_site_occupancy

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

_atom_site_adp_type

_atom_site_B_iso_or_equiv

_atom_site_type_symbol

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C3	1.0	0.144144	0.130108	0.999988	Biso	1.000000	C
C4	1.0	0.192398	0.083439	0.999979	Biso	1.000000	C
C5	1.0	0.288612	0.134050	0.000025	Biso	1.000000	C
C6	1.0	0.336036	0.085541	0.999996	Biso	1.000000	C
C7	1.0	0.431973	0.134030	0.000038	Biso	1.000000	C
C8	1.0	0.477595	0.083439	0.999984	Biso	1.000000	C
C9	1.0	0.572515	0.130096	0.999993	Biso	1.000000	C
C10	1.0	0.619024	0.080374	0.999983	Biso	1.000000	C
C11	1.0	0.714027	0.126651	0.999984	Biso	1.000000	C
C12	1.0	0.760807	0.077774	0.000003	Biso	1.000000	C
C13	1.0	0.856163	0.125825	0.000014	Biso	1.000000	C
C14	1.0	0.903469	0.077784	0.000006	Biso	1.000000	C
C15	1.0	0.999103	0.269702	0.999991	Biso	1.000000	C
C16	1.0	0.046554	0.222077	0.999983	Biso	1.000000	C
C17	1.0	0.141793	0.270861	0.999993	Biso	1.000000	C
C18	1.0	0.191818	0.226150	0.000009	Biso	1.000000	C
C19	1.0	0.288408	0.278279	0.000099	Biso	1.000000	C
C20	1.0	0.336191	0.230466	0.000146	Biso	1.000000	C
C21	1.0	0.433277	0.279995	0.000297	Biso	1.000000	C

C22	1.0	0.480807	0.230439	0.000173	Biso	1.000000	C
C23	1.0	0.576394	0.278240	0.000151	Biso	1.000000	C
C24	1.0	0.620869	0.226123	0.000032	Biso	1.000000	C
C25	1.0	0.715575	0.270829	0.000004	Biso	1.000000	C
C26	1.0	0.762027	0.222050	0.999975	Biso	1.000000	C
C27	1.0	0.857096	0.269687	0.999980	Biso	1.000000	C
C28	1.0	0.903992	0.221475	0.000003	Biso	1.000000	C
C29	1.0	0.999862	0.413269	0.999979	Biso	1.000000	C
C30	1.0	0.046650	0.365107	0.999982	Biso	1.000000	C
C31	1.0	0.141445	0.413568	0.999979	Biso	1.000000	C
C32	1.0	0.188732	0.365974	0.000004	Biso	1.000000	C
C33	1.0	0.283127	0.413397	0.000066	Biso	1.000000	C
C34	1.0	0.716718	0.413360	0.000134	Biso	1.000000	C
C35	1.0	0.763689	0.365935	0.000023	Biso	1.000000	C
C36	1.0	0.858554	0.413532	0.999964	Biso	1.000000	C
C37	1.0	0.904915	0.365091	0.999967	Biso	1.000000	C
C38	1.0	0.000818	0.556945	0.999968	Biso	1.000000	C
C39	1.0	0.047591	0.508763	0.999980	Biso	1.000000	C
C40	1.0	0.142544	0.556974	0.999984	Biso	1.000000	C
C41	1.0	0.188918	0.508546	0.999978	Biso	1.000000	C
C42	1.0	0.283796	0.556188	0.000003	Biso	1.000000	C
C43	1.0	0.330801	0.508807	0.000068	Biso	1.000000	C
C44	1.0	0.764391	0.508775	0.000137	Biso	1.000000	C
C45	1.0	0.858765	0.556155	0.000026	Biso	1.000000	C
C46	1.0	0.906015	0.508511	0.999963	Biso	1.000000	C
C47	1.0	0.000962	0.700021	0.999981	Biso	1.000000	C
C48	1.0	0.048383	0.652367	0.999985	Biso	1.000000	C
C49	1.0	0.143502	0.700614	0.000009	Biso	1.000000	C
C50	1.0	0.190386	0.652398	0.999995	Biso	1.000000	C
C51	1.0	0.285454	0.700057	0.999987	Biso	1.000000	C
C52	1.0	0.331919	0.651302	0.999994	Biso	1.000000	C
C53	1.0	0.426644	0.696063	0.000012	Biso	1.000000	C

C54	1.0	0.471137	0.643992	0.000101	Biso	1.000000	C
C55	1.0	0.566728	0.691827	0.000148	Biso	1.000000	C
C56	1.0	0.614295	0.642313	0.000296	Biso	1.000000	C
C57	1.0	0.711379	0.691797	0.000187	Biso	1.000000	C
C58	1.0	0.759150	0.643960	0.000159	Biso	1.000000	C
C59	1.0	0.855744	0.696036	0.000043	Biso	1.000000	C
C60	1.0	0.905725	0.651272	0.000011	Biso	1.000000	C
C61	1.0	0.999698	0.841755	0.999989	Biso	1.000000	C
C62	1.0	0.048394	0.795446	0.999989	Biso	1.000000	C
C63	1.0	0.144089	0.844357	0.000006	Biso	1.000000	C
C64	1.0	0.191360	0.796285	0.000019	Biso	1.000000	C
C65	1.0	0.286725	0.844381	0.000009	Biso	1.000000	C
C66	1.0	0.333473	0.795473	0.999996	Biso	1.000000	C
C67	1.0	0.428477	0.841771	0.999990	Biso	1.000000	C
C68	1.0	0.475021	0.792097	0.999990	Biso	1.000000	C
C69	1.0	0.569946	0.838781	0.999982	Biso	1.000000	C
C70	1.0	0.615581	0.788229	0.000031	Biso	1.000000	C
C71	1.0	0.711526	0.836709	0.000005	Biso	1.000000	C
C72	1.0	0.758959	0.788205	0.000053	Biso	1.000000	C
C73	1.0	0.855180	0.838756	0.999995	Biso	1.000000	C
C74	1.0	0.903434	0.792075	0.000004	Biso	1.000000	C
C75	1.0	0.999606	0.984413	0.999985	Biso	1.000000	C
C76	1.0	0.047984	0.937723	0.999983	Biso	1.000000	C
C77	1.0	0.144193	0.987373	0.999974	Biso	1.000000	C
C78	1.0	0.192128	0.940145	0.999988	Biso	1.000000	C
C79	1.0	0.287927	0.989337	0.999976	Biso	1.000000	C
C80	1.0	0.334540	0.940168	0.999987	Biso	1.000000	C
C81	1.0	0.429709	0.987381	0.999973	Biso	1.000000	C
C82	1.0	0.476218	0.937729	0.999983	Biso	1.000000	C
C83	1.0	0.571282	0.984419	0.999980	Biso	1.000000	C
C84	1.0	0.617834	0.934816	0.999975	Biso	1.000000	C
C85	1.0	0.713008	0.982021	0.999989	Biso	1.000000	C

C86	1.0	0.759648	0.932891	0.999982	Biso	1.000000 C
C87	1.0	0.855456	0.982027	0.999991	Biso	1.000000 C
C88	1.0	0.903401	0.934803	0.999979	Biso	1.000000 C
N1	1.0	0.332706	0.371353	0.000151	Biso	1.000000 N
N2	1.0	0.477871	0.369195	0.000479	Biso	1.000000 N
N3	1.0	0.625129	0.371307	0.000243	Biso	1.000000 N
N4	1.0	0.422413	0.550913	0.000153	Biso	1.000000 N
N5	1.0	0.569750	0.553122	0.000480	Biso	1.000000 N
N6	1.0	0.714858	0.550882	0.000248	Biso	1.000000 N
Co1	1.0	0.458569	0.461126	0.000385	Biso	1.000000 Co
Co2	1.0	0.589123	0.461210	0.000470	Biso	1.000000 Co

$NiNiN_6$-gra

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CRYSTAL DATA

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_chemical_name_common 'TM2 '

_cell_length_a 17.22000

_cell_length_b 17.22000

_cell_length_c 15.03910

_cell_angle_alpha 90

_cell_angle_beta 90

_cell_angle_gamma 120

_space_group_name_H-M_alt 'P 1'

_space_group_IT_number 1

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_space_group_symop_operation_xyz
  'x, y, z'

loop_
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  _atom_site_occupancy
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_adp_type
  _atom_site_B_iso_or_equiv
  _atom_site_type_symbol
  C1     1.0   0.998509   0.125976   0.999998   Biso  1.000000 C
  C2     1.0   0.047411   0.079936   0.999982   Biso  1.000000 C
  C3     1.0   0.143711   0.129993   0.000003   Biso  1.000000 C
  C4     1.0   0.192851   0.084276   0.000009   Biso  1.000000 C
  C5     1.0   0.289429   0.135716   0.000053   Biso  1.000000 C
  C6     1.0   0.336757   0.086957   0.000047   Biso  1.000000 C
  C7     1.0   0.432836   0.135725   0.000070   Biso  1.000000 C
  C8     1.0   0.477984   0.084300   0.000023   Biso  1.000000 C
  C9     1.0   0.572829   0.129996   0.000011   Biso  1.000000 C
  C10    1.0   0.619043   0.079929   0.999984   Biso  1.000000 C
  C11    1.0   0.713967   0.125973   0.999993   Biso  1.000000 C
  C12    1.0   0.760502   0.076832   0.999992   Biso  1.000000 C
  C13    1.0   0.855763   0.125036   0.000011   Biso  1.000000 C
  C14    1.0   0.902807   0.076826   0.000000   Biso  1.000000 C
  C15    1.0   0.998541   0.269182   0.999986   Biso  1.000000 C
  C16    1.0   0.045675   0.221394   0.999999   Biso  1.000000 C
  C17    1.0   0.140761   0.270378   0.000009   Biso  1.000000 C
  C18    1.0   0.190868   0.225812   0.000039   Biso  1.000000 C
  C19    1.0   0.287397   0.278342   0.000109   Biso  1.000000 C
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C20	1.0	0.337209	0.232378	0.000127	Biso	1.000000	C
C21	1.0	0.435463	0.284472	0.000241	Biso	1.000000	C
C22	1.0	0.481654	0.232380	0.000166	Biso	1.000000	C
C23	1.0	0.577418	0.278307	0.000180	Biso	1.000000	C
C24	1.0	0.621456	0.225805	0.000065	Biso	1.000000	C
C25	1.0	0.716110	0.270377	0.000020	Biso	1.000000	C
C26	1.0	0.762201	0.221386	0.999994	Biso	1.000000	C
C27	1.0	0.857116	0.269177	0.999976	Biso	1.000000	C
C28	1.0	0.903627	0.220769	0.999990	Biso	1.000000	C
C29	1.0	0.999833	0.413223	0.999952	Biso	1.000000	C
C30	1.0	0.045935	0.364712	0.999975	Biso	1.000000	C
C31	1.0	0.140312	0.413511	0.999995	Biso	1.000000	C
C32	1.0	0.186860	0.365527	0.000017	Biso	1.000000	C
C33	1.0	0.280600	0.413103	0.000081	Biso	1.000000	C
C34	1.0	0.718920	0.413083	0.000146	Biso	1.000000	C
C35	1.0	0.765118	0.365533	0.000027	Biso	1.000000	C
C36	1.0	0.859646	0.413522	0.999983	Biso	1.000000	C
C37	1.0	0.905215	0.364710	0.999959	Biso	1.000000	C
C38	1.0	0.001566	0.557398	0.999959	Biso	1.000000	C
C39	1.0	0.047650	0.508875	0.999953	Biso	1.000000	C
C40	1.0	0.142257	0.557384	0.999976	Biso	1.000000	C
C41	1.0	0.187825	0.508598	0.999997	Biso	1.000000	C
C42	1.0	0.282347	0.556615	0.000021	Biso	1.000000	C
C43	1.0	0.328548	0.509091	0.000084	Biso	1.000000	C
C44	1.0	0.766901	0.509071	0.000140	Biso	1.000000	C
C45	1.0	0.860641	0.556599	0.000027	Biso	1.000000	C
C46	1.0	0.907193	0.508614	0.999983	Biso	1.000000	C
C47	1.0	0.001871	0.700711	0.999997	Biso	1.000000	C
C48	1.0	0.048993	0.652921	0.999975	Biso	1.000000	C
C49	1.0	0.143910	0.701350	0.999989	Biso	1.000000	C
C50	1.0	0.190366	0.652910	0.999987	Biso	1.000000	C
C51	1.0	0.285281	0.700728	0.000001	Biso	1.000000	C

C52	1.0	0.331361	0.651759	0.000013	Biso	1.000000	C
C53	1.0	0.426028	0.696355	0.000049	Biso	1.000000	C
C54	1.0	0.470081	0.643911	0.000120	Biso	1.000000	C
C55	1.0	0.565873	0.689875	0.000124	Biso	1.000000	C
C56	1.0	0.612076	0.637828	0.000232	Biso	1.000000	C
C57	1.0	0.710335	0.689879	0.000153	Biso	1.000000	C
C58	1.0	0.760130	0.643879	0.000172	Biso	1.000000	C
C59	1.0	0.856668	0.696334	0.000068	Biso	1.000000	C
C60	1.0	0.906775	0.651748	0.000021	Biso	1.000000	C
C61	1.0	0.000147	0.842177	0.999986	Biso	1.000000	C
C62	1.0	0.049060	0.796140	0.999997	Biso	1.000000	C
C63	1.0	0.144771	0.845322	0.999994	Biso	1.000000	C
C64	1.0	0.191818	0.797110	0.000009	Biso	1.000000	C
C65	1.0	0.287087	0.845336	0.000001	Biso	1.000000	C
C66	1.0	0.333570	0.796153	0.999999	Biso	1.000000	C
C67	1.0	0.428505	0.842204	0.999984	Biso	1.000000	C
C68	1.0	0.474718	0.792166	0.000007	Biso	1.000000	C
C69	1.0	0.569581	0.837913	0.000012	Biso	1.000000	C
C70	1.0	0.614731	0.786514	0.000054	Biso	1.000000	C
C71	1.0	0.710812	0.835258	0.000047	Biso	1.000000	C
C72	1.0	0.758150	0.786521	0.000064	Biso	1.000000	C
C73	1.0	0.854720	0.837901	0.000024	Biso	1.000000	C
C74	1.0	0.903846	0.792149	0.000015	Biso	1.000000	C
C75	1.0	0.999286	0.984045	0.999982	Biso	1.000000	C
C76	1.0	0.048278	0.938080	0.999983	Biso	1.000000	C
C77	1.0	0.144659	0.988188	0.999988	Biso	1.000000	C
C78	1.0	0.192743	0.941144	0.999985	Biso	1.000000	C
C79	1.0	0.288579	0.990603	0.000002	Biso	1.000000	C
C80	1.0	0.334956	0.941154	0.999990	Biso	1.000000	C
C81	1.0	0.430080	0.988211	0.999993	Biso	1.000000	C
C82	1.0	0.476313	0.938101	0.999980	Biso	1.000000	C
C83	1.0	0.571254	0.984053	0.999982	Biso	1.000000	C

C84	1.0	0.617515	0.933990	0.999990	Biso	1.000000 C
C85	1.0	0.712639	0.981037	0.999985	Biso	1.000000 C
C86	1.0	0.759003	0.931594	0.000004	Biso	1.000000 C
C87	1.0	0.854823	0.981019	0.999991	Biso	1.000000 C
C88	1.0	0.902917	0.933980	0.999996	Biso	1.000000 C
N1	1.0	0.329383	0.370713	0.000130	Biso	1.000000 N
N2	1.0	0.480021	0.373690	0.000368	Biso	1.000000 N
N3	1.0	0.627760	0.370672	0.000252	Biso	1.000000 N
N4	1.0	0.419713	0.551552	0.000135	Biso	1.000000 N
N5	1.0	0.567491	0.548603	0.000362	Biso	1.000000 N
N6	1.0	0.718155	0.551513	0.000245	Biso	1.000000 N
Ni1	1.0	0.449376	0.461220	0.000207	Biso	1.000000 Ni
Ni2	1.0	0.598182	0.461110	0.000343	Biso	1.000000 Ni

$FeCoN_6$-gra

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CRYSTAL DATA

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_chemical_name_common 'TM2 '

_cell_length_a 17.22000

_cell_length_b 17.22000

_cell_length_c 15.03910

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_cell_angle_gamma 120

_space_group_name_H-M_alt 'P 1'

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  _atom_site_fract_x
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  _atom_site_B_iso_or_equiv
  _atom_site_type_symbol
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  C2     1.0    0.047965    0.080455    -0.000003    Biso  1.000000 C
  C3     1.0    0.144120    0.130099    -0.000010    Biso  1.000000 C
  C4     1.0    0.192326    0.083316    -0.000028    Biso  1.000000 C
  C5     1.0    0.288378    0.133681     0.000019    Biso  1.000000 C
  C6     1.0    0.335958    0.085369    -0.000021    Biso  1.000000 C
  C7     1.0    0.431846    0.133713     0.000035    Biso  1.000000 C
  C8     1.0    0.477557    0.083332    -0.000026    Biso  1.000000 C
  C9     1.0    0.572507    0.130028    -0.000005    Biso  1.000000 C
  C10    1.0    0.619020    0.080424    -0.000013    Biso  1.000000 C
  C11    1.0    0.714061    0.126730    -0.000013    Biso  1.000000 C
  C12    1.0    0.760904    0.077952     0.000010    Biso  1.000000 C
  C13    1.0    0.856223    0.125879     0.000015    Biso  1.000000 C
  C14    1.0    0.903582    0.077979     0.000008    Biso  1.000000 C
  C15    1.0   -0.000865    0.269725    -0.000006    Biso  1.000000 C
  C16    1.0    0.046611    0.222183    -0.000017    Biso  1.000000 C
  C17    1.0    0.141801    0.270918    -0.000006    Biso  1.000000 C
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C19	1.0	0.288343	0.278248	0.000087	Biso	1.000000	C
C20	1.0	0.336123	0.230229	0.000148	Biso	1.000000	C
C21	1.0	0.432662	0.279137	0.000293	Biso	1.000000	C
C22	1.0	0.480683	0.230269	0.000188	Biso	1.000000	C
C23	1.0	0.576351	0.278022	0.000139	Biso	1.000000	C
C24	1.0	0.620831	0.226103	0.000029	Biso	1.000000	C
C25	1.0	0.715647	0.270855	-0.000005	Biso	1.000000	C
C26	1.0	0.762076	0.222184	-0.000030	Biso	1.000000	C
C27	1.0	0.857184	0.269724	-0.000013	Biso	1.000000	C
C28	1.0	0.904040	0.221558	0.000011	Biso	1.000000	C
C29	1.0	-0.000084	0.413254	-0.000012	Biso	1.000000	C
C30	1.0	0.046687	0.365134	-0.000014	Biso	1.000000	C
C31	1.0	0.141454	0.413577	-0.000024	Biso	1.000000	C
C32	1.0	0.188741	0.366001	0.000000	Biso	1.000000	C
C33	1.0	0.283024	0.413400	0.000053	Biso	1.000000	C
C34	1.0	0.717114	0.413437	0.000124	Biso	1.000000	C
C35	1.0	0.763816	0.365998	0.000014	Biso	1.000000	C
C36	1.0	0.858739	0.413575	-0.000052	Biso	1.000000	C
C37	1.0	0.905042	0.365124	-0.000033	Biso	1.000000	C
C38	1.0	0.000917	0.556920	-0.000033	Biso	1.000000	C
C39	1.0	0.047666	0.508794	-0.000012	Biso	1.000000	C
C40	1.0	0.142551	0.556934	-0.000014	Biso	1.000000	C
C41	1.0	0.188917	0.508536	-0.000026	Biso	1.000000	C
C42	1.0	0.283788	0.556159	-0.000001	Biso	1.000000	C
C43	1.0	0.330714	0.508820	0.000055	Biso	1.000000	C
C44	1.0	0.764702	0.508700	0.000123	Biso	1.000000	C
C45	1.0	0.858826	0.556074	0.000016	Biso	1.000000	C
C46	1.0	0.906164	0.508472	-0.000052	Biso	1.000000	C
C47	1.0	0.000857	0.699873	-0.000030	Biso	1.000000	C
C48	1.0	0.048429	0.652332	-0.000014	Biso	1.000000	C
C49	1.0	0.143461	0.700527	0.000011	Biso	1.000000	C

C50	1.0	0.190382	0.652350	-0.000005	Biso	1.000000	C
C51	1.0	0.285407	0.699934	-0.000017	Biso	1.000000	C
C52	1.0	0.331887	0.651239	-0.000007	Biso	1.000000	C
C53	1.0	0.426649	0.696031	0.000001	Biso	1.000000	C
C54	1.0	0.471125	0.644041	0.000092	Biso	1.000000	C
C55	1.0	0.566925	0.692091	0.000165	Biso	1.000000	C
C56	1.0	0.614540	0.643184	0.000310	Biso	1.000000	C
C57	1.0	0.711436	0.691985	0.000201	Biso	1.000000	C
C58	1.0	0.759334	0.644189	0.000144	Biso	1.000000	C
C59	1.0	0.855733	0.696057	0.000033	Biso	1.000000	C
C60	1.0	0.905752	0.651222	-0.000003	Biso	1.000000	C
C61	1.0	-0.000346	0.841710	-0.000011	Biso	1.000000	C
C62	1.0	0.048342	0.795357	-0.000013	Biso	1.000000	C
C63	1.0	0.143994	0.844175	0.000011	Biso	1.000000	C
C64	1.0	0.191345	0.796237	0.000015	Biso	1.000000	C
C65	1.0	0.286623	0.844196	0.000009	Biso	1.000000	C
C66	1.0	0.333442	0.795369	-0.000006	Biso	1.000000	C
C67	1.0	0.428493	0.841697	-0.000002	Biso	1.000000	C
C68	1.0	0.475007	0.792096	-0.000009	Biso	1.000000	C
C69	1.0	0.569999	0.838881	-0.000026	Biso	1.000000	C
C70	1.0	0.615724	0.788608	0.000024	Biso	1.000000	C
C71	1.0	0.711615	0.836880	-0.000019	Biso	1.000000	C
C72	1.0	0.759145	0.788528	0.000039	Biso	1.000000	C
C73	1.0	0.855240	0.838858	-0.000024	Biso	1.000000	C
C74	1.0	0.903500	0.792144	-0.000002	Biso	1.000000	C
C75	1.0	-0.000347	0.984455	-0.000011	Biso	1.000000	C
C76	1.0	0.047980	0.937715	-0.000014	Biso	1.000000	C
C77	1.0	0.144101	0.987219	-0.000025	Biso	1.000000	C
C78	1.0	0.192078	0.940008	-0.000003	Biso	1.000000	C
C79	1.0	0.287782	0.989009	-0.000025	Biso	1.000000	C
C80	1.0	0.334472	0.940028	-0.000004	Biso	1.000000	C
C81	1.0	0.429657	0.987218	-0.000026	Biso	1.000000	C

C82	1.0	0.476222	0.937701	-0.000010	Biso	1.000000 C
C83	1.0	0.571292	0.984437	-0.000014	Biso	1.000000 C
C84	1.0	0.617885	0.934950	-0.000024	Biso	1.000000 C
C85	1.0	0.713088	0.982143	-0.000004	Biso	1.000000 C
C86	1.0	0.759827	0.933206	-0.000025	Biso	1.000000 C
C87	1.0	0.855540	0.982165	-0.000007	Biso	1.000000 C
C88	1.0	0.903527	0.934965	-0.000027	Biso	1.000000 C
N1	1.0	0.332684	0.371341	0.000164	Biso	1.000000 N
N2	1.0	0.477770	0.368756	0.000505	Biso	1.000000 N
N3	1.0	0.625132	0.371314	0.000223	Biso	1.000000 N
N4	1.0	0.422425	0.550937	0.000167	Biso	1.000000 N
N5	1.0	0.570070	0.553570	0.000524	Biso	1.000000 N
N6	1.0	0.714844	0.550878	0.000222	Biso	1.000000 N
Fe1	1.0	0.457643	0.461136	0.000456	Biso	1.000000 Fe
Co1	1.0	0.588147	0.461195	0.000536	Biso	1.000000 Co

$FeNiN_6$-gra

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CRYSTAL DATA

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data_VESTA_phase_1

_chemical_name_common 'TM2 '

_cell_length_a 17.22000

_cell_length_b 17.22000

_cell_length_c 15.03910

_cell_angle_alpha 90

_cell_angle_beta 90

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_space_group_IT_number                 1

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  _atom_site_occupancy
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_adp_type
  _atom_site_B_iso_or_equiv
  _atom_site_type_symbol
  C1        1.0   -0.000459     0.127134     0.000004     Biso  1.000000 C
  C2        1.0    0.048232     0.080659    -0.000015     Biso  1.000000 C
  C3        1.0    0.144395     0.130001    -0.000022     Biso  1.000000 C
  C4        1.0    0.192403     0.082956    -0.000028     Biso  1.000000 C
  C5        1.0    0.288481     0.133491    -0.000064     Biso  1.000000 C
  C6        1.0    0.335652     0.084823    -0.000036     Biso  1.000000 C
  C7        1.0    0.431602     0.133694    -0.000042     Biso  1.000000 C
  C8        1.0    0.477115     0.082942    -0.000020     Biso  1.000000 C
  C9        1.0    0.572099     0.129942    -0.000025     Biso  1.000000 C
  C10       1.0    0.618908     0.080603    -0.000008     Biso  1.000000 C
  C11       1.0    0.714076     0.127151     0.000003     Biso  1.000000 C
  C12       1.0    0.761300     0.078689     0.000002     Biso  1.000000 C
  C13       1.0    0.856770     0.126970    -0.000001     Biso  1.000000 C
  C14       1.0    0.903862     0.078655     0.000004     Biso  1.000000 C
  C15       1.0   -0.000459     0.270427     0.000006     Biso  1.000000 C
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C16	1.0	0.046987	0.222610	-0.000012	Biso	1.000000	C
C17	1.0	0.142097	0.270907	-0.000034	Biso	1.000000	C
C18	1.0	0.192027	0.225986	0.000023	Biso	1.000000	C
C19	1.0	0.288274	0.277910	0.000080	Biso	1.000000	C
C20	1.0	0.336322	0.230099	0.000011	Biso	1.000000	C
C21	1.0	0.433017	0.280639	0.000362	Biso	1.000000	C
C22	1.0	0.480260	0.230407	0.000104	Biso	1.000000	C
C23	1.0	0.576133	0.277627	0.000114	Biso	1.000000	C
C24	1.0	0.620538	0.225907	-0.000017	Biso	1.000000	C
C25	1.0	0.715353	0.270982	-0.000030	Biso	1.000000	C
C26	1.0	0.762188	0.222682	-0.000003	Biso	1.000000	C
C27	1.0	0.857489	0.270432	0.000005	Biso	1.000000	C
C28	1.0	0.904539	0.222650	0.000006	Biso	1.000000	C
C29	1.0	0.000098	0.413525	0.000014	Biso	1.000000	C
C30	1.0	0.046936	0.365574	-0.000008	Biso	1.000000	C
C31	1.0	0.141506	0.413640	-0.000055	Biso	1.000000	C
C32	1.0	0.188544	0.365971	-0.000016	Biso	1.000000	C
C33	1.0	0.282407	0.413231	0.000131	Biso	1.000000	C
C34	1.0	0.717856	0.413379	0.000084	Biso	1.000000	C
C35	1.0	0.764289	0.366071	-0.000081	Biso	1.000000	C
C36	1.0	0.859017	0.413859	-0.000074	Biso	1.000000	C
C37	1.0	0.905326	0.365547	-0.000002	Biso	1.000000	C
C38	1.0	0.000913	0.556693	-0.000001	Biso	1.000000	C
C39	1.0	0.047698	0.508728	0.000014	Biso	1.000000	C
C40	1.0	0.142474	0.556659	-0.000010	Biso	1.000000	C
C41	1.0	0.188848	0.508453	-0.000059	Biso	1.000000	C
C42	1.0	0.283533	0.556120	-0.000017	Biso	1.000000	C
C43	1.0	0.330183	0.508930	0.000137	Biso	1.000000	C
C44	1.0	0.765578	0.508798	0.000082	Biso	1.000000	C
C45	1.0	0.859329	0.556162	-0.000081	Biso	1.000000	C
C46	1.0	0.906286	0.508375	-0.000070	Biso	1.000000	C
C47	1.0	0.000537	0.699496	-0.000004	Biso	1.000000	C

C48	1.0	0.048145	0.651777	0.000005	Biso	1.000000 C
C49	1.0	0.143014	0.699544	0.000007	Biso	1.000000 C
C50	1.0	0.190269	0.651782	0.000005	Biso	1.000000 C
C51	1.0	0.285520	0.699509	-0.000014	Biso	1.000000 C
C52	1.0	0.332183	0.651150	-0.000035	Biso	1.000000 C
C53	1.0	0.427023	0.696265	0.000030	Biso	1.000000 C
C54	1.0	0.471280	0.644362	0.000100	Biso	1.000000 C
C55	1.0	0.567221	0.692170	0.000010	Biso	1.000000 C
C56	1.0	0.613557	0.641695	0.000356	Biso	1.000000 C
C57	1.0	0.711018	0.691903	0.000108	Biso	1.000000 C
C58	1.0	0.759512	0.644486	0.000120	Biso	1.000000 C
C59	1.0	0.855584	0.696239	-0.000014	Biso	1.000000 C
C60	1.0	0.905422	0.651233	-0.000030	Biso	1.000000 C
C61	1.0	-0.000768	0.841451	-0.000008	Biso	1.000000 C
C62	1.0	0.047936	0.794998	0.000003	Biso	1.000000 C
C63	1.0	0.143617	0.843393	0.000002	Biso	1.000000 C
C64	1.0	0.190902	0.795208	-0.000002	Biso	1.000000 C
C65	1.0	0.286317	0.843397	0.000004	Biso	1.000000 C
C66	1.0	0.333527	0.794940	0.000004	Biso	1.000000 C
C67	1.0	0.428666	0.841411	-0.000015	Biso	1.000000 C
C68	1.0	0.475464	0.792210	-0.000020	Biso	1.000000 C
C69	1.0	0.570509	0.839248	-0.000029	Biso	1.000000 C
C70	1.0	0.616050	0.788823	-0.000065	Biso	1.000000 C
C71	1.0	0.711864	0.837351	-0.000037	Biso	1.000000 C
C72	1.0	0.759006	0.788577	-0.000039	Biso	1.000000 C
C73	1.0	0.855134	0.839183	-0.000017	Biso	1.000000 C
C74	1.0	0.903101	0.792178	-0.000021	Biso	1.000000 C
C75	1.0	-0.000338	0.984594	0.000001	Biso	1.000000 C
C76	1.0	0.047711	0.937452	0.000004	Biso	1.000000 C
C77	1.0	0.143970	0.986700	0.000009	Biso	1.000000 C
C78	1.0	0.191704	0.939148	0.000007	Biso	1.000000 C
C79	1.0	0.287419	0.988229	-0.000000	Biso	1.000000 C

C80	1.0	0.333970	0.939100	0.000005	Biso	1.000000 C
C81	1.0	0.429276	0.986700	0.000008	Biso	1.000000 C
C82	1.0	0.476215	0.937459	0.000001	Biso	1.000000 C
C83	1.0	0.571381	0.984602	0.000005	Biso	1.000000 C
C84	1.0	0.618365	0.935423	0.000008	Biso	1.000000 C
C85	1.0	0.713601	0.982891	0.000006	Biso	1.000000 C
C86	1.0	0.760187	0.933855	-0.000002	Biso	1.000000 C
C87	1.0	0.855794	0.982942	0.000005	Biso	1.000000 C
C88	1.0	0.903490	0.935378	0.000008	Biso	1.000000 C
N1	1.0	0.330751	0.370162	0.000065	Biso	1.000000 N
N2	1.0	0.478013	0.369554	0.000792	Biso	1.000000 N
N3	1.0	0.626136	0.370278	0.000426	Biso	1.000000 N
N4	1.0	0.421599	0.552107	0.000084	Biso	1.000000 N
N5	1.0	0.569915	0.552764	0.000794	Biso	1.000000 N
N6	1.0	0.716808	0.551802	0.000415	Biso	1.000000 N
Fe1	1.0	0.452032	0.461130	0.000472	Biso	1.000000 Fe
Ni1	1.0	0.592023	0.461182	0.000467	Biso	1.000000 Ni

$CoNiN_6$-gra

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CRYSTAL DATA

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data_VESTA_phase_1

_chemical_name_common 'TM2 '

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_cell_length_b 17.22000

_cell_length_c 15.03910

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_space_group_IT_number                 1

loop_
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  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_adp_type
  _atom_site_B_iso_or_equiv
  _atom_site_type_symbol
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  C2        1.0    0.047675     0.080175     -0.000003     Biso  1.000000 C
  C3        1.0    0.143847     0.129945     -0.000000     Biso  1.000000 C
  C4        1.0    0.192489     0.083640     -0.000021     Biso  1.000000 C
  C5        1.0    0.288817     0.134485      0.000033     Biso  1.000000 C
  C6        1.0    0.336291     0.086008     -0.000008     Biso  1.000000 C
  C7        1.0    0.432263     0.134593      0.000050     Biso  1.000000 C
  C8        1.0    0.477797     0.083762     -0.000016     Biso  1.000000 C
  C9        1.0    0.572708     0.130058      0.000012     Biso  1.000000 C
  C10       1.0    0.619057     0.080253     -0.000006     Biso  1.000000 C
  C11       1.0    0.714076     0.126460     -0.000015     Biso  1.000000 C
  C12       1.0    0.760770     0.077498      0.000011     Biso  1.000000 C
  C13       1.0    0.856023     0.125488      0.000020     Biso  1.000000 C
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C14	1.0	0.903256	0.077463	0.000012	Biso	1.000000	C
C15	1.0	-0.001145	0.269478	-0.000003	Biso	1.000000	C
C16	1.0	0.046198	0.221804	-0.000020	Biso	1.000000	C
C17	1.0	0.141320	0.270644	0.000000	Biso	1.000000	C
C18	1.0	0.191241	0.225854	0.000021	Biso	1.000000	C
C19	1.0	0.287820	0.278033	0.000093	Biso	1.000000	C
C20	1.0	0.336529	0.231007	0.000164	Biso	1.000000	C
C21	1.0	0.433888	0.281535	0.000305	Biso	1.000000	C
C22	1.0	0.481091	0.231109	0.000194	Biso	1.000000	C
C23	1.0	0.576842	0.278229	0.000115	Biso	1.000000	C
C24	1.0	0.621178	0.226036	0.000043	Biso	1.000000	C
C25	1.0	0.715855	0.270660	0.000013	Biso	1.000000	C
C26	1.0	0.762147	0.221808	-0.000032	Biso	1.000000	C
C27	1.0	0.857177	0.269467	-0.000017	Biso	1.000000	C
C28	1.0	0.903859	0.221196	0.000016	Biso	1.000000	C
C29	1.0	-0.000153	0.413186	-0.000014	Biso	1.000000	C
C30	1.0	0.046316	0.364905	-0.000017	Biso	1.000000	C
C31	1.0	0.140930	0.413522	-0.000030	Biso	1.000000	C
C32	1.0	0.187861	0.365804	0.000018	Biso	1.000000	C
C33	1.0	0.281956	0.413257	0.000080	Biso	1.000000	C
C34	1.0	0.717852	0.413265	0.000121	Biso	1.000000	C
C35	1.0	0.764359	0.365800	0.000041	Biso	1.000000	C
C36	1.0	0.859107	0.413545	-0.000038	Biso	1.000000	C
C37	1.0	0.905128	0.364943	-0.000036	Biso	1.000000	C
C38	1.0	0.001202	0.557106	-0.000036	Biso	1.000000	C
C39	1.0	0.047659	0.508846	-0.000015	Biso	1.000000	C
C40	1.0	0.142396	0.557133	-0.000019	Biso	1.000000	C
C41	1.0	0.188444	0.508569	-0.000030	Biso	1.000000	C
C42	1.0	0.283086	0.556356	0.000021	Biso	1.000000	C
C43	1.0	0.329799	0.508979	0.000082	Biso	1.000000	C
C44	1.0	0.765617	0.508866	0.000126	Biso	1.000000	C
C45	1.0	0.859572	0.556282	0.000045	Biso	1.000000	C

C46	1.0	0.906578	0.508540	-0.000040	Biso	1.000000	C
C47	1.0	0.001328	0.700251	-0.000033	Biso	1.000000	C
C48	1.0	0.048696	0.652598	-0.000018	Biso	1.000000	C
C49	1.0	0.143654	0.700880	0.000016	Biso	1.000000	C
C50	1.0	0.190341	0.652576	-0.000004	Biso	1.000000	C
C51	1.0	0.285346	0.700306	-0.000019	Biso	1.000000	C
C52	1.0	0.331671	0.651521	0.000005	Biso	1.000000	C
C53	1.0	0.426371	0.696347	0.000029	Biso	1.000000	C
C54	1.0	0.470838	0.644255	0.000100	Biso	1.000000	C
C55	1.0	0.566564	0.691300	0.000171	Biso	1.000000	C
C56	1.0	0.613388	0.640788	0.000311	Biso	1.000000	C
C57	1.0	0.711005	0.691137	0.000202	Biso	1.000000	C
C58	1.0	0.759629	0.643988	0.000125	Biso	1.000000	C
C59	1.0	0.856155	0.696114	0.000048	Biso	1.000000	C
C60	1.0	0.906166	0.651429	0.000017	Biso	1.000000	C
C61	1.0	-0.000148	0.841871	-0.000007	Biso	1.000000	C
C62	1.0	0.048643	0.795634	-0.000016	Biso	1.000000	C
C63	1.0	0.144341	0.844631	0.000011	Biso	1.000000	C
C64	1.0	0.191574	0.796627	0.000022	Biso	1.000000	C
C65	1.0	0.286842	0.844705	0.000013	Biso	1.000000	C
C66	1.0	0.333506	0.795726	-0.000006	Biso	1.000000	C
C67	1.0	0.428488	0.841992	-0.000001	Biso	1.000000	C
C68	1.0	0.474879	0.792240	0.000006	Biso	1.000000	C
C69	1.0	0.569827	0.838551	-0.000020	Biso	1.000000	C
C70	1.0	0.615345	0.787774	0.000033	Biso	1.000000	C
C71	1.0	0.711298	0.836234	-0.000009	Biso	1.000000	C
C72	1.0	0.758679	0.787645	0.000052	Biso	1.000000	C
C73	1.0	0.855059	0.838433	-0.000013	Biso	1.000000	C
C74	1.0	0.903664	0.792100	0.000014	Biso	1.000000	C
C75	1.0	-0.000539	0.984204	-0.000011	Biso	1.000000	C
C76	1.0	0.048094	0.937836	-0.000013	Biso	1.000000	C
C77	1.0	0.144343	0.987614	-0.000023	Biso	1.000000	C

C78	1.0	0.192384	0.940460	-0.000002	Biso	1.000000 C
C79	1.0	0.288101	0.989644	-0.000020	Biso	1.000000 C
C80	1.0	0.334675	0.940510	-0.000004	Biso	1.000000 C
C81	1.0	0.429877	0.987716	-0.000025	Biso	1.000000 C
C82	1.0	0.476290	0.937961	-0.000010	Biso	1.000000 C
C83	1.0	0.571288	0.984310	-0.000012	Biso	1.000000 C
C84	1.0	0.617727	0.934544	-0.000023	Biso	1.000000 C
C85	1.0	0.712936	0.981704	-0.000003	Biso	1.000000 C
C86	1.0	0.759494	0.932568	-0.000020	Biso	1.000000 C
C87	1.0	0.855237	0.981683	-0.000003	Biso	1.000000 C
C88	1.0	0.903243	0.934477	-0.000024	Biso	1.000000 C
N1	1.0	0.330751	0.370572	0.000119	Biso	1.000000 N
N2	1.0	0.479590	0.370692	0.000488	Biso	1.000000 N
N3	1.0	0.626320	0.371146	0.000155	Biso	1.000000 N
N4	1.0	0.421267	0.551715	0.000122	Biso	1.000000 N
N5	1.0	0.569924	0.551658	0.000485	Biso	1.000000 N
N6	1.0	0.716240	0.551071	0.000172	Biso	1.000000 N
Co1	1.0	0.452784	0.461131	0.000358	Biso	1.000000 Co
Ni1	1.0	0.592769	0.461245	0.000395	Biso	1.000000 Ni

Notes and references

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