Supporting Information

Nitrogen doped graphene on transition metal substrates as efficient bifunctional catalysts for oxygen reduction and oxygen evolution reactions

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S1. Zero-point energy and entropic correction

Table S1. Zero-point energy (ZPE) and entropic correction (TS) at T = 298 K for relevant species in ORR and OER. The values of H_2O, H_2 and O_2 molecules are taken from the NIST-JANAF thermodynamics table.[1] The vibrational frequencies of OH*, OOH* and O* species are calculated on selected C sites of the NG–Co(111) and NG–Fe(110) models, and they give similar results for ZPE and TS. Thus, constant values of ZPE and TS are used for the oxygenated intermediates adsorbed on various C sites of our model structures.

Species	ZPE (eV)	TS (eV)
H_2O	0.56	0.67
H_2	0.27	0.41
O_2	0.11	0.64
OH*	0.36	0.06
OOH*	0.40	0.08
O*	0.05	0

S2. Model structures of N-doped graphene on transition metals

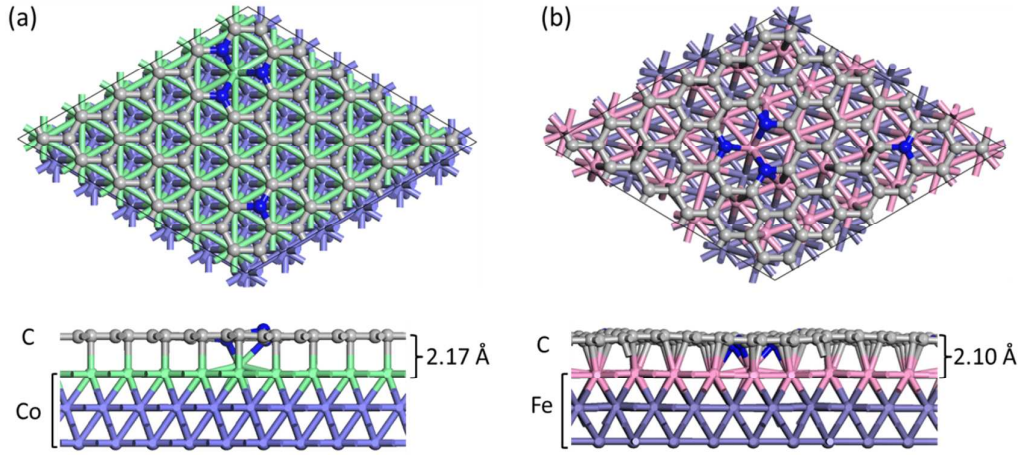

Figure S1. Model structures of N-doped graphene on (a) Co(111) and (b) Fe(110) substrates, where the N atoms are on (or close to) the hollow site of the metal substrates. The C, N, Co and Fe atoms are shown in silver, blue, green and pink colors, respectively. The bottom layers of Co and Fe atoms are shown in medium and dark blue colors for clear view, respectively.

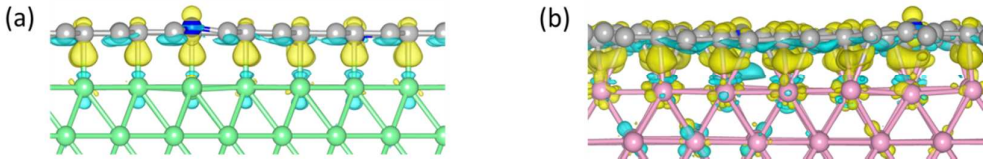

Figure S2. Side views of differential charge densities of N-doped graphene on (a) Co(111) and (b) Fe(110) substrates, where the N atoms are on (or close to) the top site of the metal substrates. The C, N, Co and Fe atoms are shown in silver, blue, green and pink colors, respectively. The yellow and cyan colors represent electron accumulation and depletion regions with isosurface value of 0.005 e/Å^3.

S3. Scaling relation of binding energies of intermediates

The binding energies of OH* and OOH* species adsorbed on the NG–Co(111) and NG–Fe(110) heterostructures follows the linear correlation $\Delta E_{OH^*} = \Delta E_{OOH^*} - 3.18$ eV, which sets upper limits for the overpotentials of ORR and OER. Consider the four-electron reaction pathway for ORR in alkaline media:

$$* + O_2\ (g) + H_2O\ (l) + e^- \rightarrow OOH^* + OH^- \quad (1)$$

$$OOH^* + e^- \rightarrow O^* + OH^- \quad (2)$$

$$O^* + H_2O\ (l) + e^- \rightarrow OH^* + OH^- \quad (3)$$

$$OH^* + e^- \rightarrow * + OH^- \quad (4)$$

Using the relation

$$G(OH^-) - G(e^-) = G(H_2O) - 1/2G(H_2) + k_BT\cdot\ln10\cdot PH \quad (5)$$

The Gibbs free energy of formation for the 2nd and 3rd step can be written as

$$\Delta G_2 + \Delta G_3 = G(OH^*) - G(OOH^*) + G(H_2O) - G(H_2) + 2k_BT\cdot\ln10\cdot PH \quad (6)$$

where $G(OH^*)$, $G(OOH^*)$, $G(H_2O)$ and $G(H_2)$ are the Gibbs free energies of OH* and OOH* species, and H_2O and H_2 molecules, respectively. By including the zero-point energy and entropic correction given by Table S1, there is

$$\Delta G_2 + \Delta G_3 = \Delta E_{OH^*} - \Delta E_{OOH^*} + 1.62 = -1.56\ eV \quad (7)$$

which uses the scaling constant $\Delta E_{OH^*} - \Delta E_{OOH^*} = -3.18$ eV from the linear correlation. As the Gibbs free energy of formation for the overall ORR process is

$$\Delta G = \Delta G_1 + \Delta G_2 + \Delta G_3 + \Delta G_4 = -1.61\ eV \quad (8)$$

there is also a constraint

$$\Delta G_1 + \Delta G_4 = (-1.61) - (-1.56) = -0.05\ eV \quad (9)$$

The lowest overpotential for ORR is achieved by equally splitting the constrained potential $\Delta G_1 = \Delta G_4$, giving

$$\eta^{ORR} = \Delta G_{max}/e + U_0 = -0.05/2 + 0.40 = 0.38\ V \quad (10)$$

For OER, the lowest overpotential is attained at $\Delta G_2 = \Delta G_3$, yielding

$$\eta^{OER} = \Delta G_{max}/e - U_0 = 1.56/2 - 0.40 = 0.38\ V \quad (11)$$

The critical value for ΔE_{OH^*} can be obtained from eq 4 and eq 5:

$$\Delta G_4 = G(OH^-) - G(e^-) - G(OH^*) = -\Delta E_{OH^*} + 0.54 \quad (12)$$

At $\Delta G_1 = \Delta G_4 = -0.025$ eV, there are $\Delta E_{OH^*} = 0.56$ eV and $\Delta E_{OOH^*} = 3.74$ eV. The critical binding energy for OER can be calculated from eq 2 and eq 5:

$$\Delta G_2 = G(\mathrm{OOH^*}) - G(\mathrm{O^*}) + G(e^-) - G(\mathrm{OH^-}) = \Delta E_{OOH^*} - \Delta E_{O^*} - 0.52 \text{ eV} \qquad (13)$$

At $\Delta G_2 = \Delta G_3 = 0.78$ eV, there is $\Delta E_{OOH^*} - \Delta E_{O^*} = 1.30$ eV. These critical values are the optimum binding strength for the oxygenated intermediates to achieve the best catalytic activities for ORR and OER.

S4. Overpotentials of freestanding N-doped graphene

Table S2. Binding energies of oxygenated intermediates (ΔE_{OH*}, ΔE_{OOH*} and ΔE_{O*}), ORR and OER overpotentials (η^{ORR} and η^{OER}) and partial charge for various types of C sites in freestanding N-doped graphene as shown in Figure S3.

site	ΔE_{OH*} (eV)	ΔE_{OOH*} (eV)	ΔE_{O*} (eV)	η^{ORR} (V)	η^{OER} (V)	charge (e)
1 (C−N_1)	1.34	4.60	2.88	1.24	0.80	0.15
1' (C−N_2)	2.17	5.33	3.89	1.97	1.28	0.18
2 (C_m−$2N_2$)	1.45	4.63	3.17	1.27	0.56	−0.02
2' (C_m−N)	1.96	5.12	3.19	1.76	1.07	−0.01
3 (C−C)	2.28	5.44	3.37	2.07	1.39	0

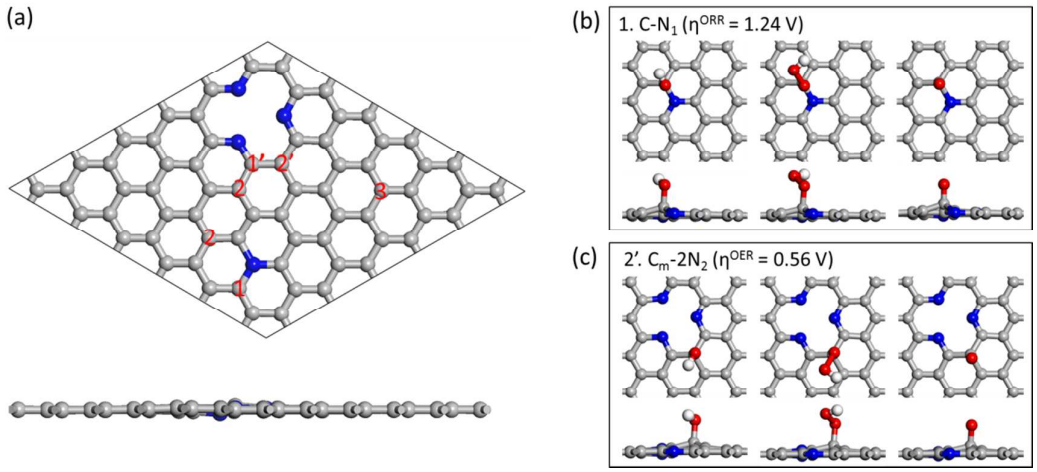

Figure S3. (a) Atomic structure of freestanding N-doped graphene of (6 × 6) unit cell. The red numbers indicate various types of C sites, for which the binding energies of oxygenated intermediates and the ORR and OER overpotentials are calculated and reported in Table S2. (b), (c) Atomic structures of oxygenated intermediates adsorbed on the type 1 and type 2' C sites, respectively. The H, C, N and O atoms are shown in white, silver, blue and red colors, respectively.

S5. Overpotentials of NG–Co(111)

Table S3 and Figure S4 shows the structure and catalytic properties for ORR and OER for N-doped graphene on Co(111) substrate, where the N atoms are located on the hollow site. The catalytic properties are similar to those of the model with N dopants on the top site (see Figure 1a and Table 1 of the main text). The lowest overpotentials for both ORR and OER are achieved on the C atoms on the hollow site and in the meta-position of pyridinic N atoms (denoted as "H_m–N_2") with η^{ORR} = 0.53 V and η^{OER} = 0.41 V. The hollow site C atoms in the meta-position of graphitic N (denoted as "H_m–N_1") or far from N atoms (denoted as "H") provide weaker oxygen binding and give larger overpotentials η^{ORR} = 0.62~0.68 V and η^{OER} = 0.43~0.45 V. The C atoms bonded to N dopants (denoted as "C_t–N_1" and "C_t–N_2") all lie on the top site of Co substrate. They have weak oxygen binding strength and thus poor activities for ORR and OER.

Table S3. Binding energies of oxygenated intermediates (ΔE_{OH*}, ΔE_{OOH*} and ΔE_{O*}), ORR and OER overpotentials (η^{ORR} and η^{OER}) and partial charge for various types of C sites in the NG–Co(111) model as shown in Figure S4.

site	ΔE_{OH*} (eV)	ΔE_{OOH*} (eV)	ΔE_{O*} (eV)	η^{ORR} (V)	η^{OER} (V)	charge (*e*)
1 (C_t–N_1)	0.99	4.23	1.83	0.87	1.47	0
1' (C_t–N_2)	0.76	4.14	2.40	0.78	0.82	0
2 (H_m–N_1)	0.73	3.98	2.61	0.62	0.45	−0.10
2' (H_m–N_2)	0.70	3.89	2.56	0.53	0.41	−0.10
2" (H)	0.84	4.04	2.69	0.68	0.43	−0.11
3 (T_m–N)	1.10	4.35	2.49	0.99	0.94	−0.13
3' (T)	1.21	4.42	2.58	1.06	0.92	−0.15

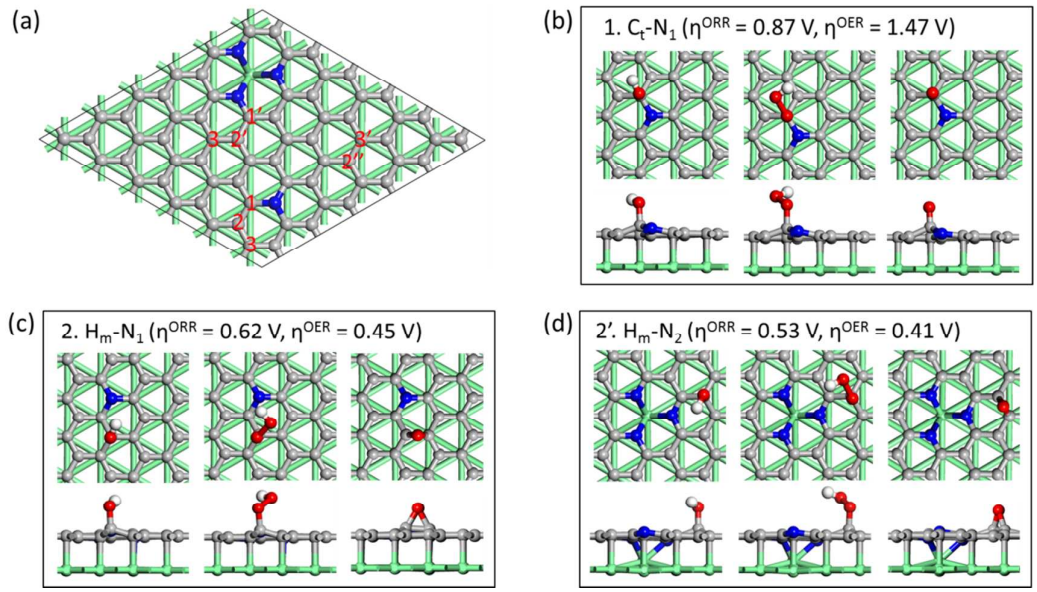

Figure S4. (a) Various types of C sites in NG–Co(111) (indicated by red numbers), for which the binding energies of oxygenated intermediates and ORR and OER overpotentials are calculated and reported in Table S3. (b), (c), (d) Atomic structures of oxygenated intermediates adsorbed on selected C sites. The H, C, N, O and Co atoms are shown in white, silver, blue, red and green colors, respectively. Only the topmost layer Co atoms in the metal substrate are displayed for clear view.

S6. Overpotentials of NG–Fe(110)

Table S4. Binding energies of oxygenated intermediates (ΔE_{OH*}, ΔE_{OOH*} and ΔE_{O*}), ORR and OER overpotentials (η^{ORR} and η^{OER}) and partial charge for selected C sites in the NG–Fe(110) models as shown in Figure S5a,b. The results for the model in Figure S5b are marked by stars.

site	ΔE_{OH*} (eV)	ΔE_{OOH*} (eV)	ΔE_{O*} (eV)	η^{ORR} (V)	η^{OER} (V)	charge (*e*)
1 (C−N_1)	0.01	3.27	1.61	0.88	0.74	0.03
1' (C−N_2)	−0.15	3.07	0.66	1.04	1.53	0.04
2 (H−N_1)	0.42	3.61	2.30	0.47	0.39	−0.12
2' (H−N_2)	0.15	3.35	1.89	0.74	0.53	−0.11
*2 (H−N_1)	0.11	3.35	2.02	0.78	0.41	−0.10
*2' (H)	0.28	3.48	2.04	0.61	0.53	−0.10
3 (M−N_1)	0.56	3.74	2.11	0.38	0.71	−0.14
3 (M−N_2)	0.41	3.64	2.35	0.48	0.37	−0.13
*3 (M)	0.45	3.69	2.14	0.44	0.62	−0.13
4 (T)	0.64	3.86	3.10	0.49	0.91	−0.15
*4 (T−N_1)	0.63	3.86	1.74	0.50	1.20	−0.15
*4' (T)	0.89	4.08	2.53	0.72	0.63	−0.16

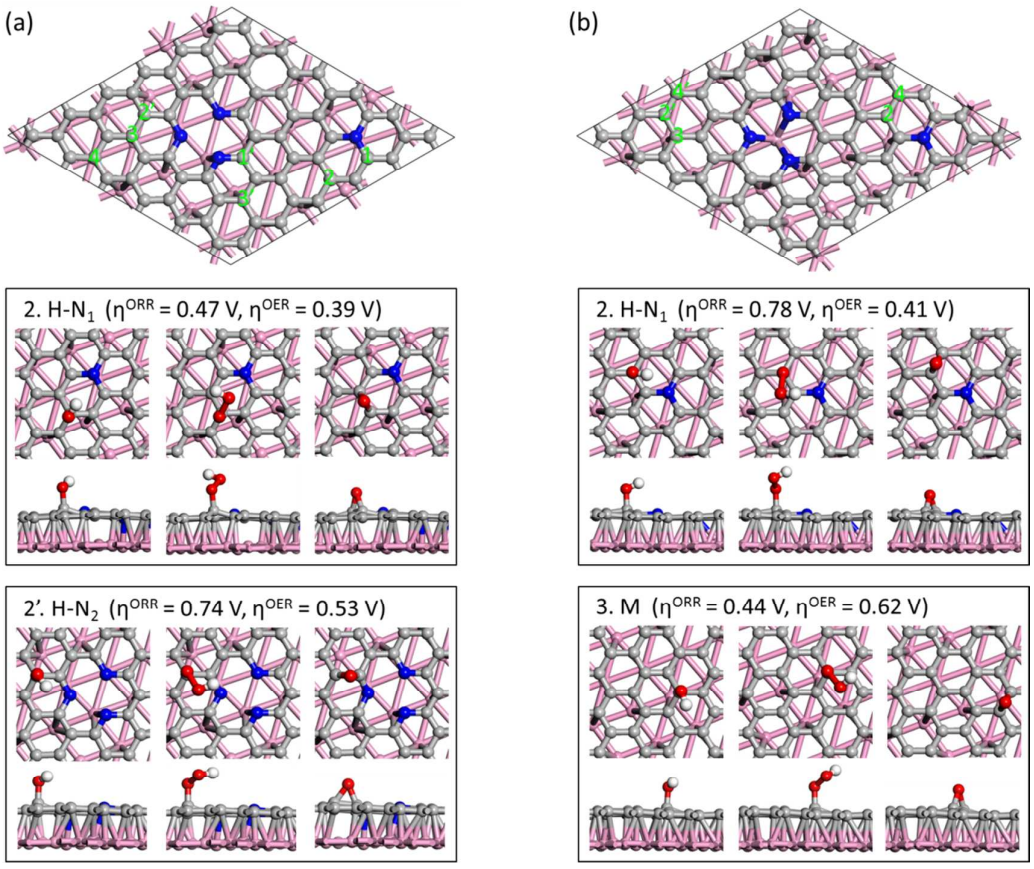

Figure S5. Model structures of NG–Fe(110) with N atoms close to the (a) top site and (b) hollow site of the Fe substrate. The green numbers indicate various types of C sites, for which the binding energies of oxygenated intermediates and ORR and OER overpotentials are calculated and reported in Table S4. Atomic structures of oxygenated intermediates adsorbed on selected C sites are shown below each model. The H, C, N, O and Fe atoms are shown in white, silver, blue, red and pink colors, respectively. Only the topmost layer Fe atoms in the metal substrate are displayed for clear view.

S7. Band decomposed charge densities of NG–Co(111) and NG–Fe(110)

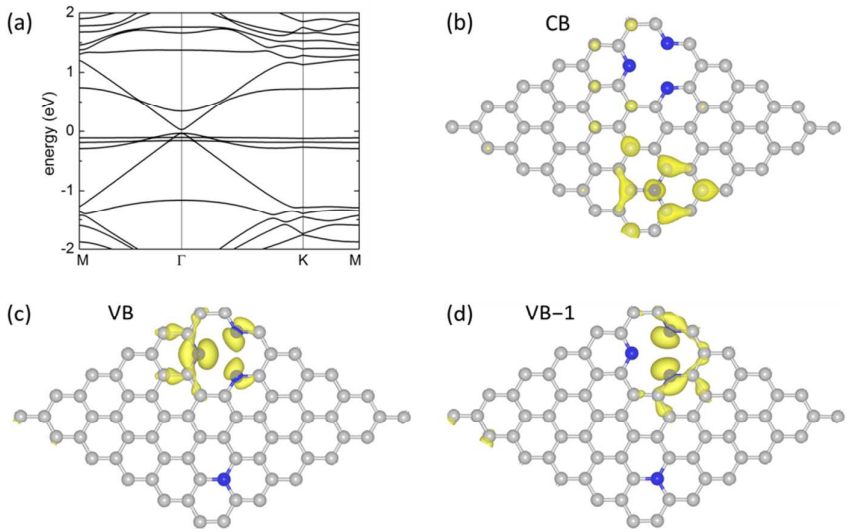

Figure S6. (a) Electronic band structure of freestanding N-doped graphene which is shown in Figure S3a. The Fermi energy is shifted to zero. (b), (c), (d) Band decomposed charge densities of the bottom conduction band (CB), top valence band (VB), and the valence band below VB (VB−1), respectively, with isosurface value of 0.005 e/Å^3. The C and N atoms are shown in silver and blue colors, respectively.

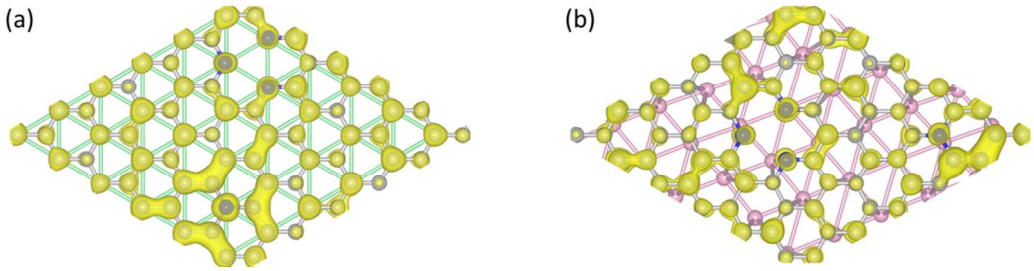

Figure S7. Band decomposed charge densities of the state across the Fermi level for (a) NG–Co(111) and (b) NG–Fe(110), with isosurface value of 0.005 e/Å^3. The C, N, Co and Fe atoms are represented in silver, blue, green and pink colors, respectively. Only the topmost layer metal atoms are shown, and only the isosurface of the graphitic sheet are displayed for clear view. The full atomic structures are given by Figure 1 of the main text.

S8. Atomic positions of NG–Co(111) and NG–Fe(110) models

NG-Co(111) model-1

1.00000000000000

12.8864580083124523 -7.4400000000000004 0.0000000000000000

0.0000000000000000 14.8800000000000026 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Co

67 4 108

Direct

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0.5564079880301379	0.1271574934312068	0.4930585617114431
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NG-Fe(110) model-1

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0.7756629799421213	0.8277068476193619	0.5100690137490642

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