Electronic Supplementary Information

Ferrocene Units Substitution in Nickel(II) Porphyrin(2.1.2.1) Induce Extremely Low Oxygen Evolution Reaction Overpotential

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Table of Contents

1, OER DFT Calculation

Our spin-polarized density functional theory (DFT) calculations[1,2] were carried out in the CP2K code.[3] All calculations employed a mixed Gaussian and planewave basis sets. Core electrons were represented with norm-conserving Goedecker-Teter-Hutter pseudopotentials,[4-6] and the valence electron wavefunction was expanded in a double-zeta basis set with polarization functions[7] along with an auxiliary plane wave basis set with an energy cutoff of 450 eV. The generalized gradient approximation exchange-correlation functional of Perdew, Burke, and Enzerhof (PBE)[8] was used. Each configuration was optimized with the Broyden-Fletcher-Goldfarb-Shanno (BGFS) algorithm with SCF convergence criteria of 1.0×10^{-6} au. The van der Waals correction of Grimme's DFT-D3 model was also adopted[9].

The typical four-electron OER reaction mechanism was considered in this work. Under alkalinez conditions, the overall reaction can be represented as

$$4OH^- \rightarrow O_2 + 2H_2O + 4(e^-) \qquad \Delta G_0 = 4.92\ eV \qquad \text{(S1)}$$

The Gibbs free energy difference (ΔG_0) is 4.92 eV at p = 1 bar and T = 298.15 K. The reaction was generally believed to proceed in four steps[10-12]

$$OH^- \rightarrow *OH + e^- \qquad \text{(S2)}$$

$$*OH + OH^- \rightarrow *O + + H_2O + e^- \qquad \text{(S3)}$$

$$*O + OH^- \rightarrow *OOH + e^- \qquad \text{(S4)}$$

$$*OOH + OH^- \rightarrow * + O_2 + H_2O + e^- \qquad \text{(S5)}$$

where * represents the active site of the catalyst, and OOH*, O*, and OH* represent the species adsorbed on the active site. At the standard condition (p = 1 bar and T = 298.15), the Gibbs free energy of $H^+ + e^-$ equals the Gibbs free energy of 1/2 H_2. The Gibbs free reaction energy (ΔG), which is calculated by the binding strengths

between the catalyst and the OER intermediates

$$\Delta G = \Delta E + \Delta E_{ZPE} - T\Delta S \tag{S6}$$

where ΔE is the DFT calculated adsorption energy of the intermediate. Herein, ΔE of OOH*, O* and OH* intermediates are all referred to H_2O and H_2.

$$\Delta E_{OOH*} = E_{OOH*} - E_* - (2E_{H_2O} - \frac{3}{2}E_{H_2}) \tag{S7}$$

$$\Delta E_{O*} = E_{O*} - E_* - (E_{H_2O} - E_{H_2}) \tag{S8}$$

$$\Delta E_{OH*} = E_{OH*} - E_* - (E_{H_2O} - \frac{1}{2}E_{H_2}) \tag{S9}$$

where E_{H_2O} and E_{H_2} are the calculated DFT energies of H_2O and H_2 molecules using the approaches outlined by Nørskov *et al.*[10,12]

The zero-point energy (ZPE) contribution is given by:

$$E_{ZPE} = \sum_i \frac{hv_i}{2} \tag{S10}$$

where h and v_i are the Plank's constant and vibrational frequencies which are calculated based on the localized harmonic oscillator approximation with a displacement of 0.01 Å. During the frequency calculation, only the mobile ascorbates and the atoms at the active site were considered while all other atoms on the catalyst are treated as fixed. The vibrational entropy contributions (S) can be calculated below:

$$S = k_B \sum_i \left(\frac{hv_i}{k_B T\left(e^{hv_i/k_B T} - 1\right)} - ln\left(1 - e^{-hv_i/k_B T}\right) \right) \tag{S11}$$

Because the high-spin ground state of an oxygen molecule is difficult to accurately describe in DFT calculation, the Gibbs free energy of O_2(g) is derived as

$$G_{O_2} = 2G_{H_2O} - 2G_{H_2} + 4.92\ eV \quad \text{(S12)}$$

2, Supporting Figures

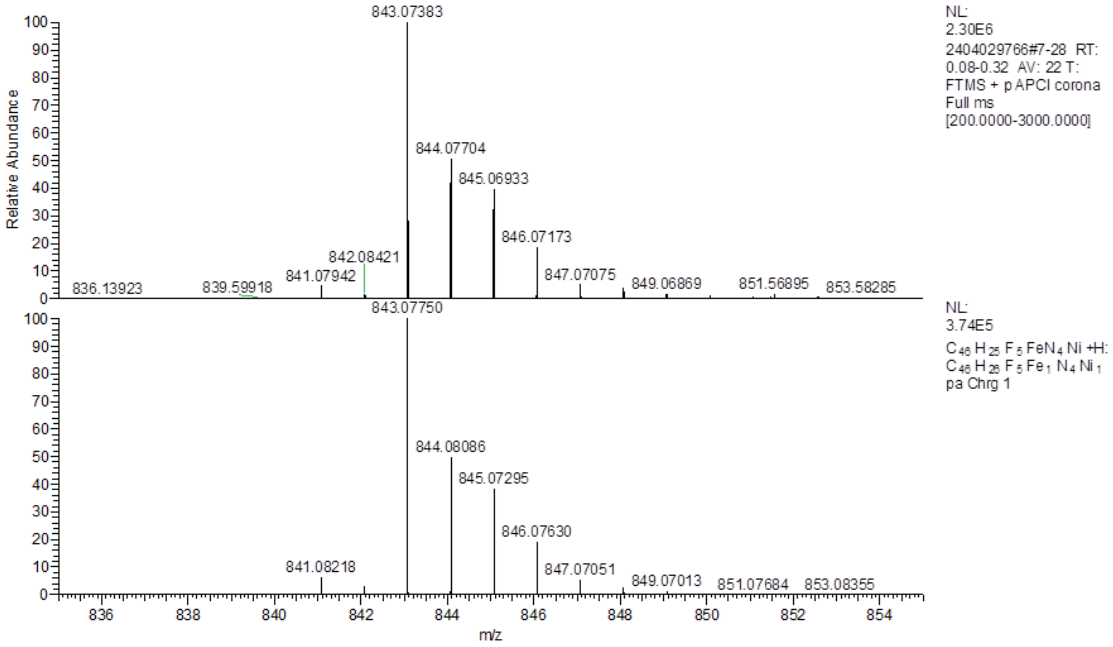

Fig. S1. HR-APCI-MS spectrum of **Ni-2**.

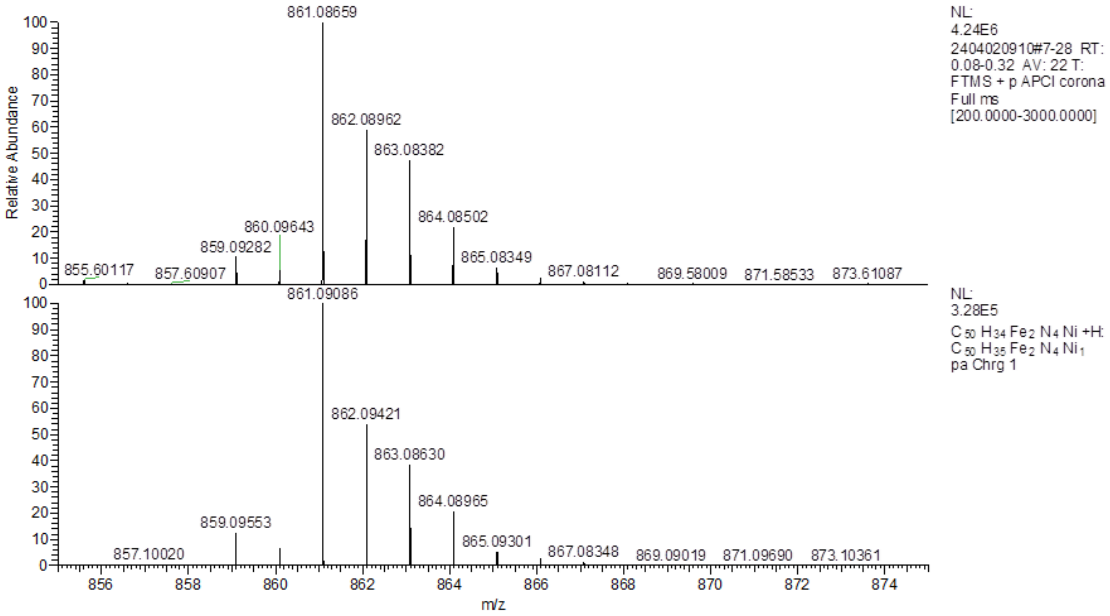

Fig. S2. HR-APCI-MS spectrum of **Ni-3**.

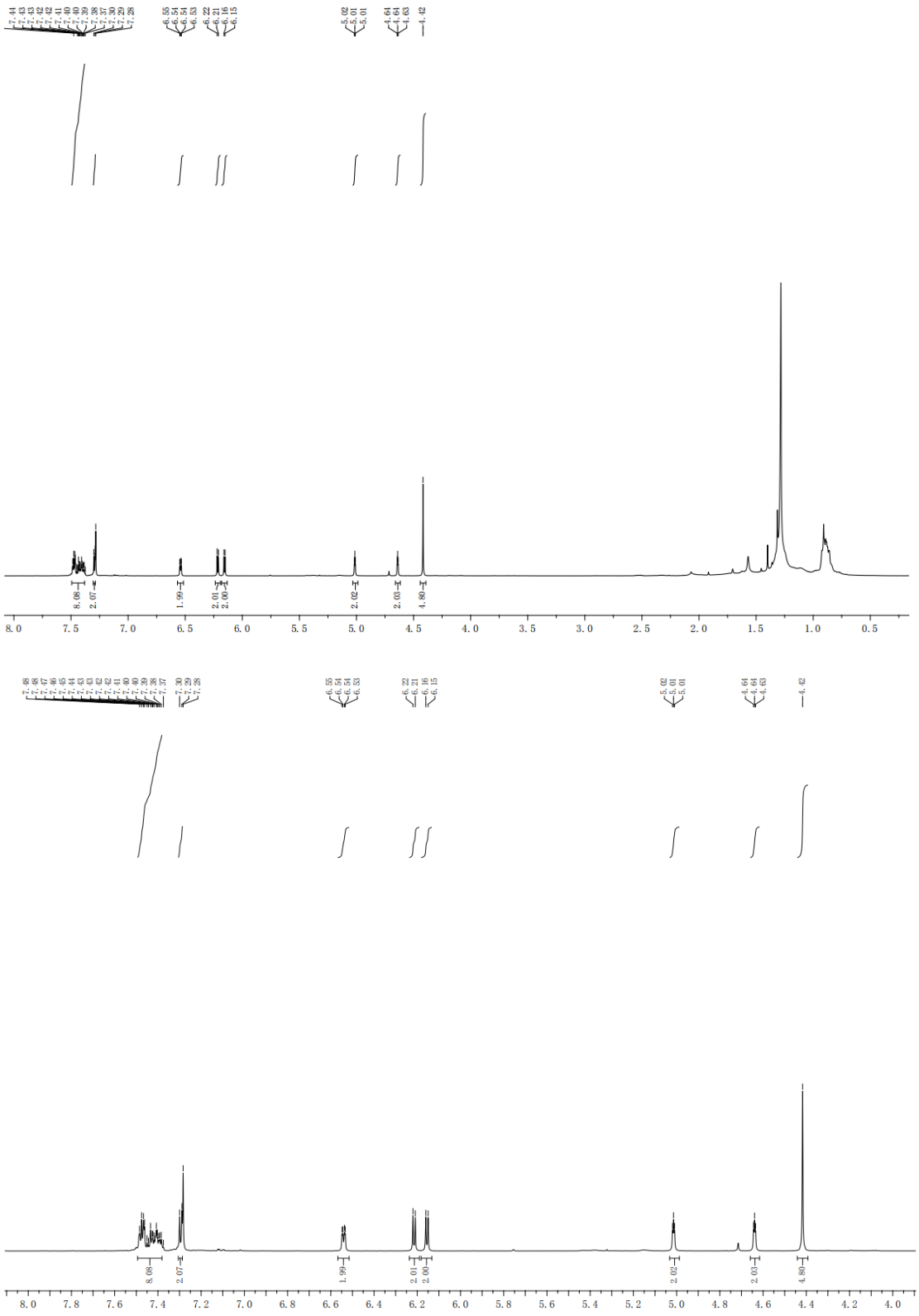

Fig. S3. ^{1}H NMR spectrum of **Ni-2** (up, from 8 – 0 ppm; bottom, from 8 – 4 ppm) in $CDCl_3$.

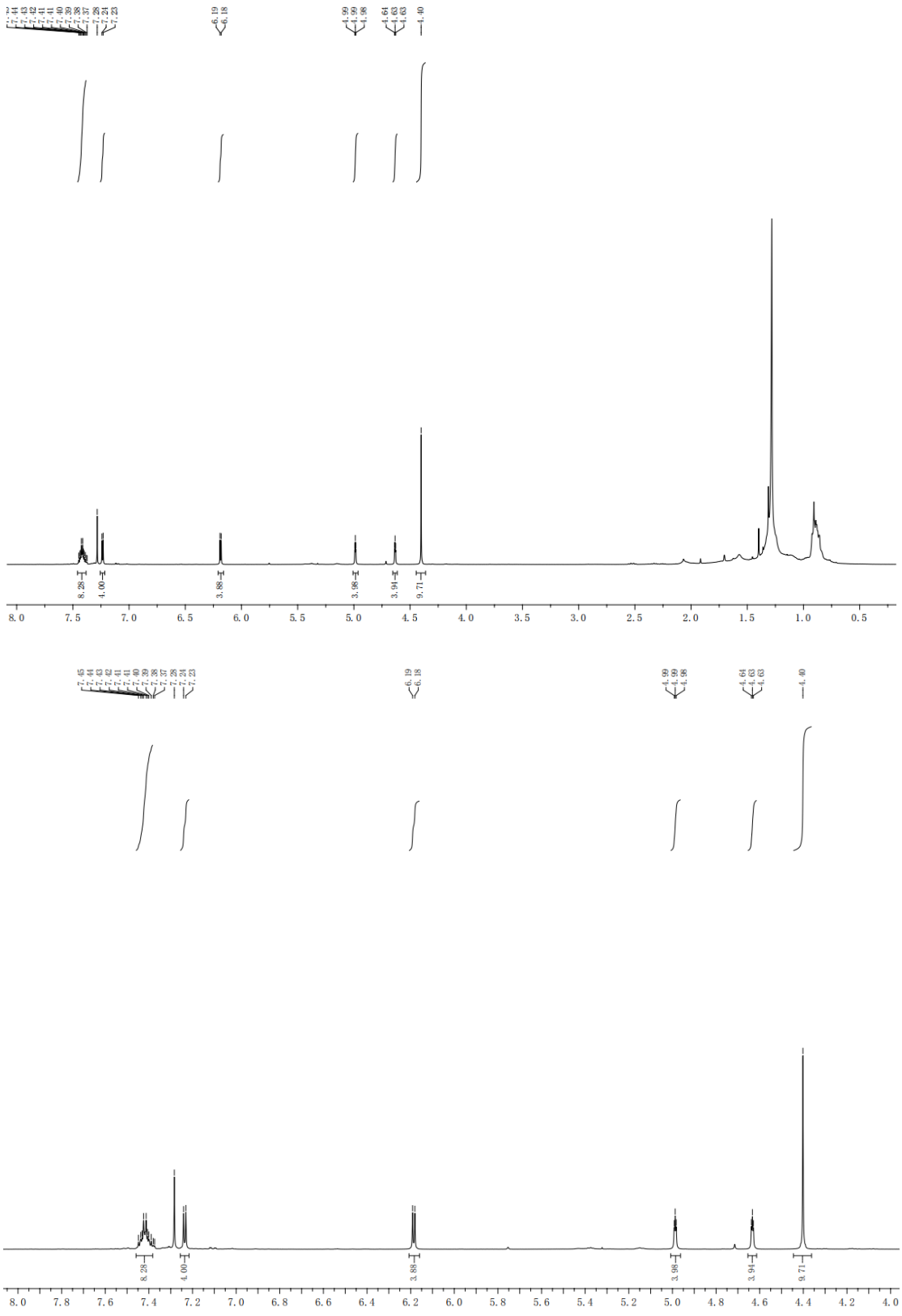

Fig. S4. ^{1}H NMR spectrum of **Ni-3** (up, from 8 – 0 ppm; bottom, from 8 – 4 ppm) in $CDCl_3$.

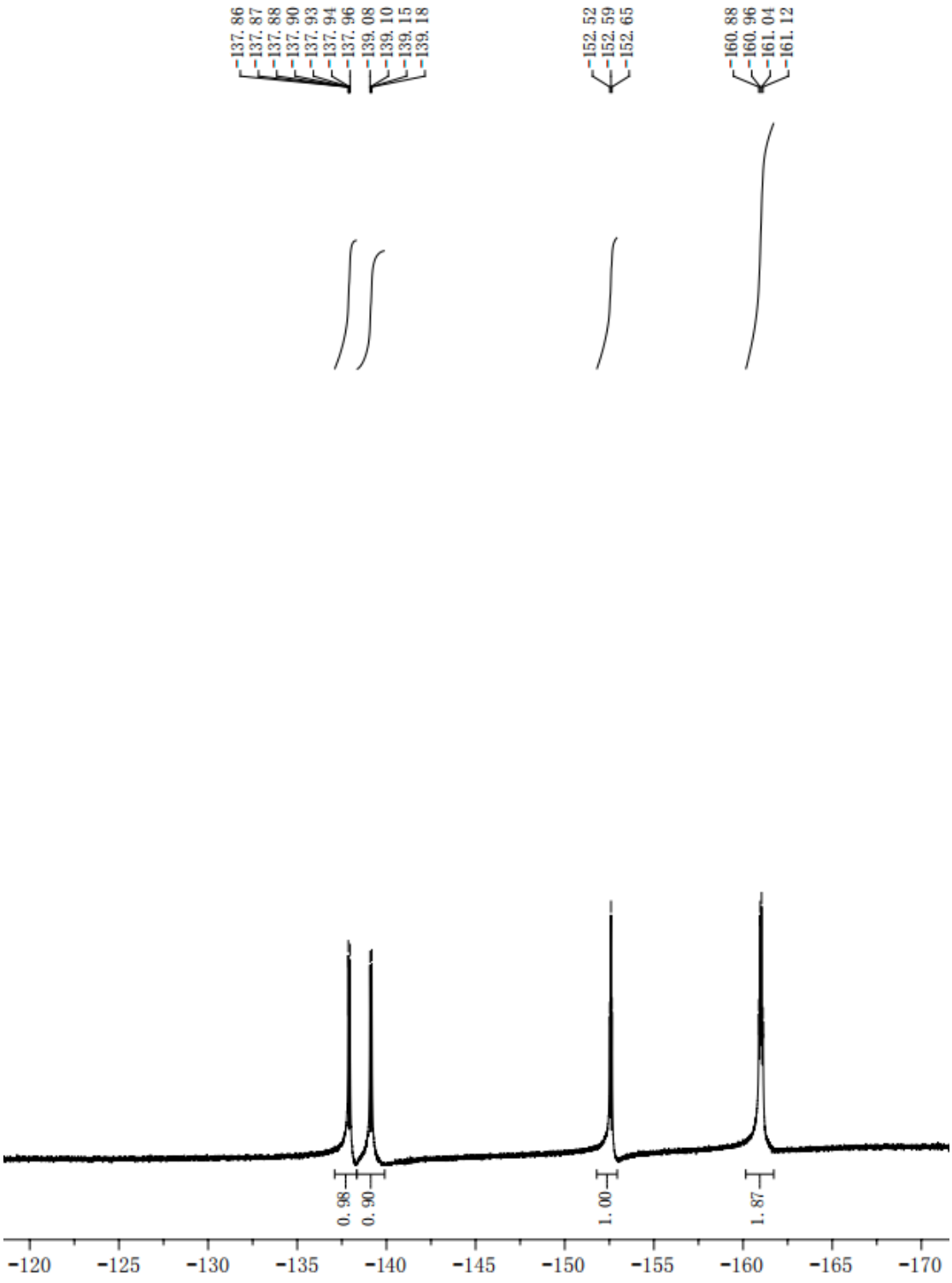

Fig. S5. ^{19}F NMR spectrum of **Ni-2** in $CDCl_3$.

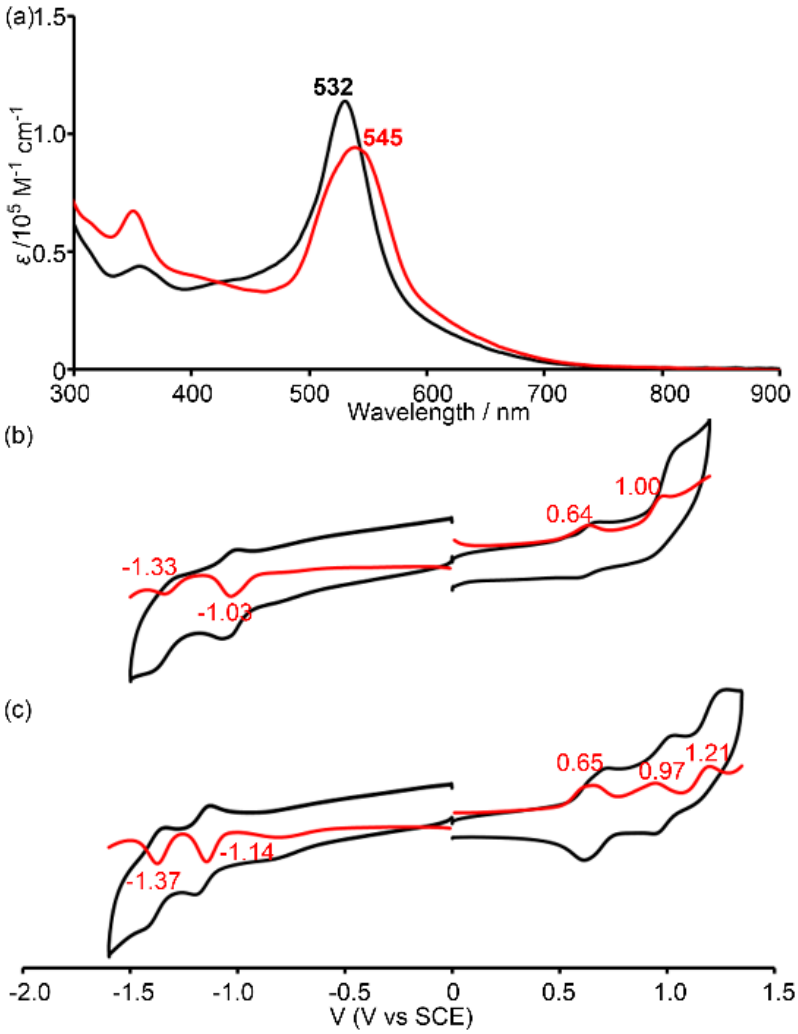

Fig. S6. (a) UV-Vis absorption spectra of **Ni-2** (black line) and **Ni-3** (red line) in CH_2Cl_2 at 293K. CVs (black line) and DPVs (red line) of (b) **Ni-2** and (c) **Ni-3** in CH_2Cl_2 containing 0.1 M TBAP. Scan rate is 0.1 V/S.

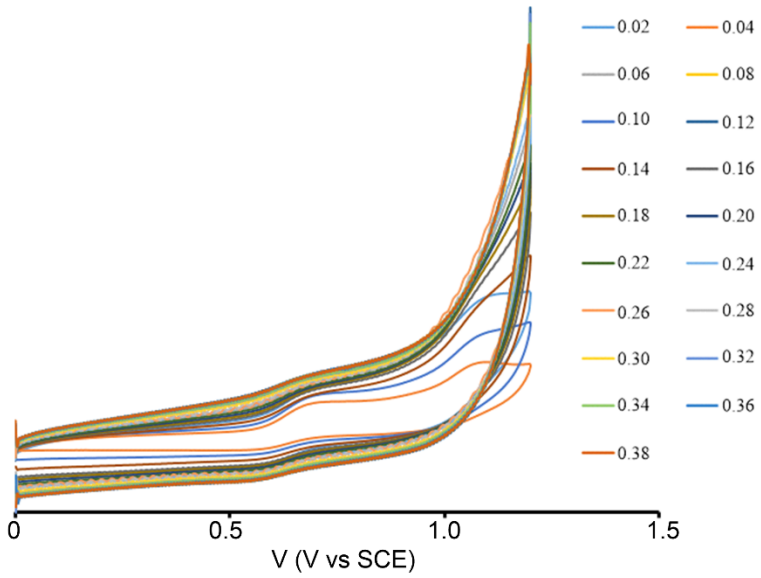

Fig. S7. The oxidation CVs of **Ni-2** in CH_2Cl_2 containing 0.1 M TBAP with different scan rate (V/S).

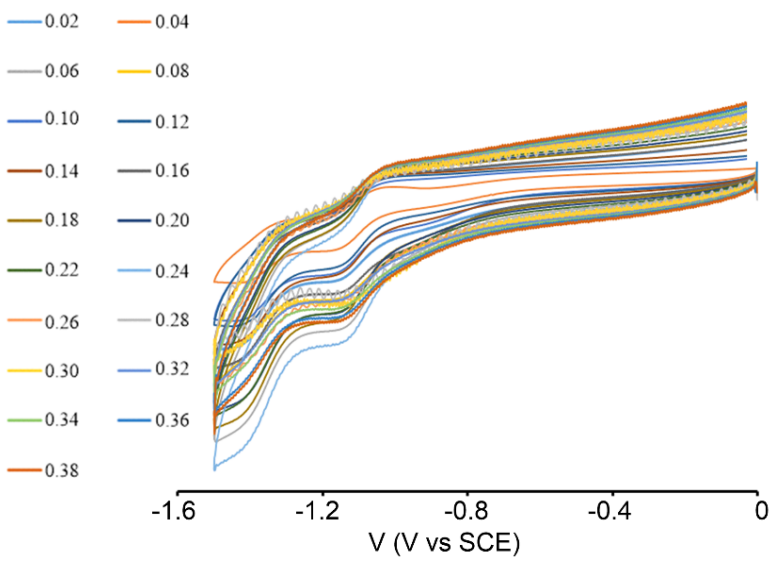

Fig. S8. The reduction CVs of **Ni-2** in CH_2Cl_2 containing 0.1 M TBAP with different scan rate (V/S).

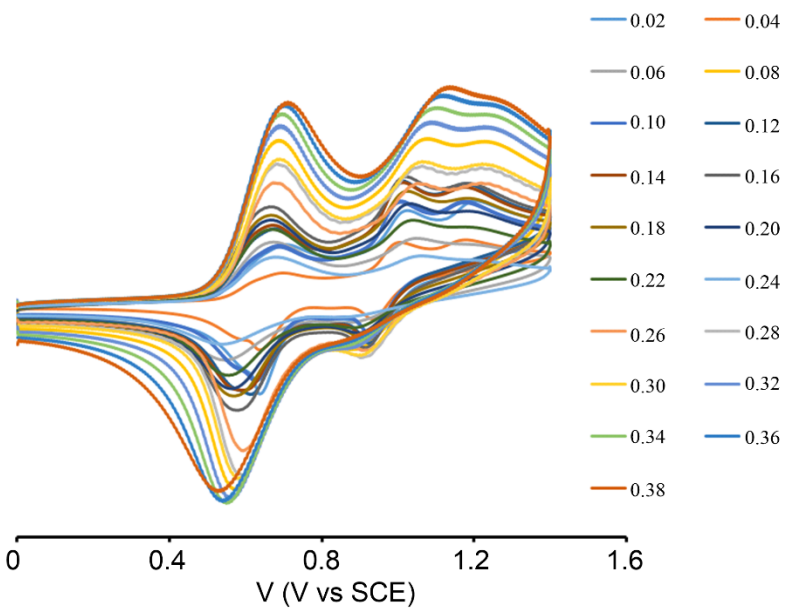

Fig. S9. The oxidation CVs of **Ni-3** in CH_2Cl_2 containing 0.1 M TBAP with different scan rate (V/S).

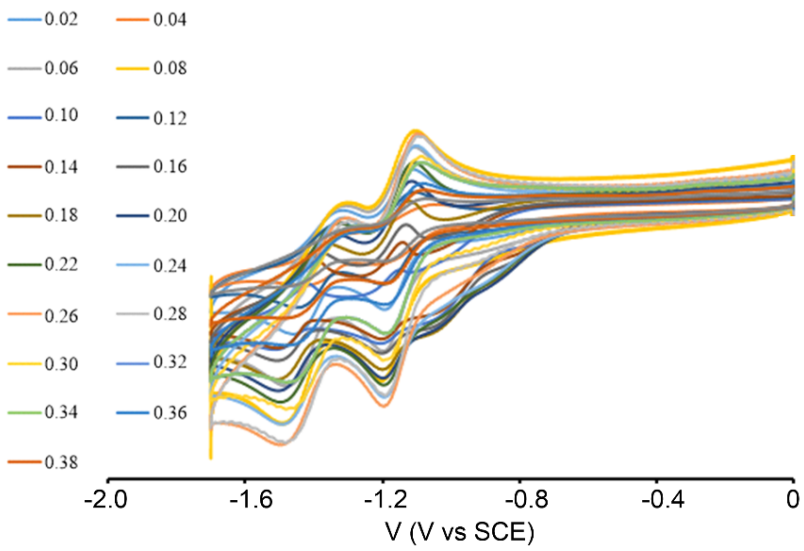

Fig. S10. The reduction CVs of **Ni-3** in CH_2Cl_2 containing 0.1 M TBAP with different scan rate (V/S).

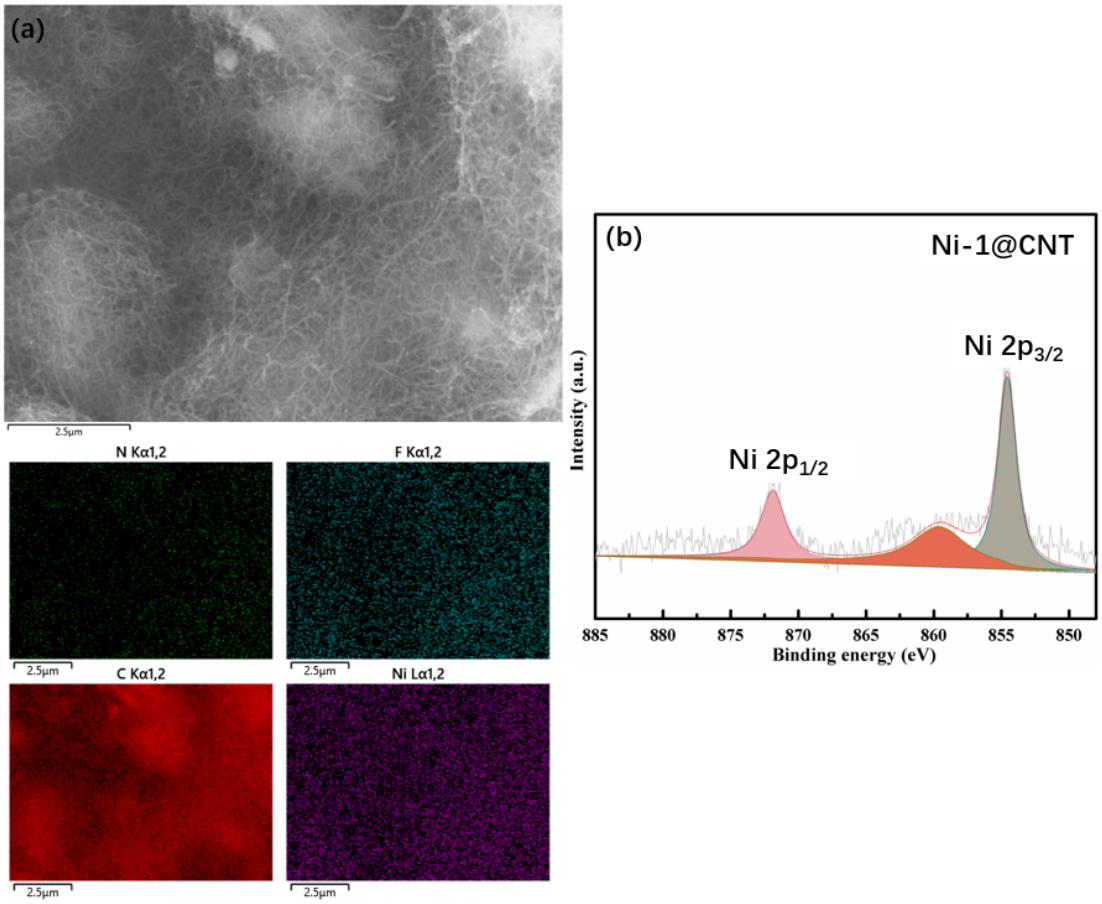

Fig. S11. (a) SEM image of **Ni-1**@CNT and the EDS elemental mapping images. (b) The corresponding Ni 2p and Fe 2p binding energy region of XPS scan spectrum of **Ni-1**@CNT.

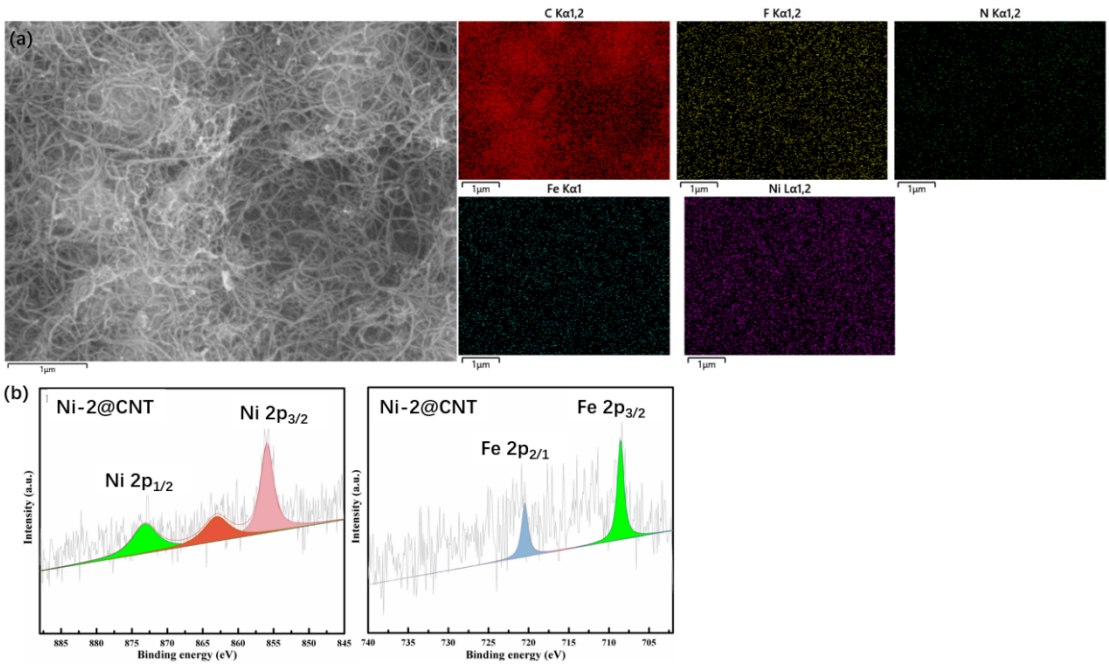

Fig. S12. (a) SEM image of **Ni-2**@CNT and the EDS elemental mapping images. (b) The corresponding Ni 2p and Fe 2p binding energy region of XPS scan spectrum of **Ni-2**@CNT.

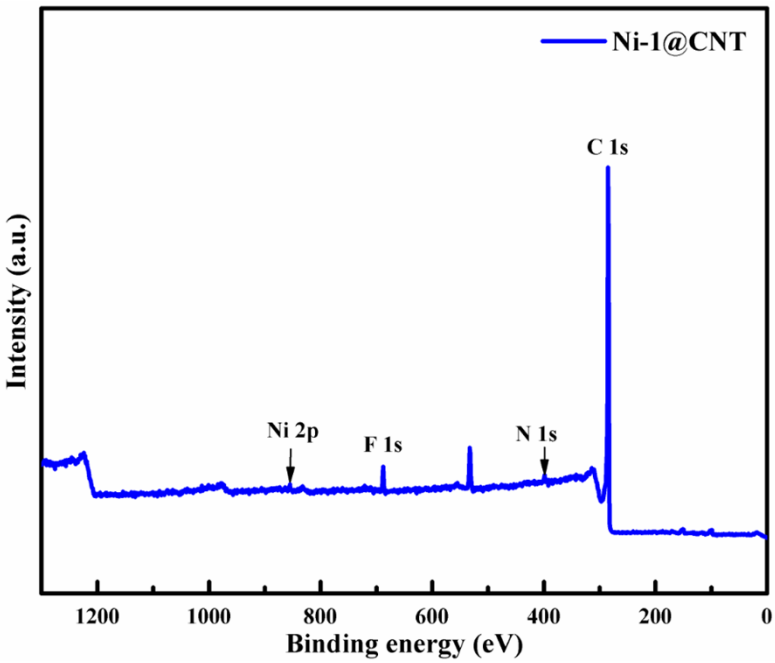

Fig. S13. XPS scan spectrum of **Ni-1@**CNT.

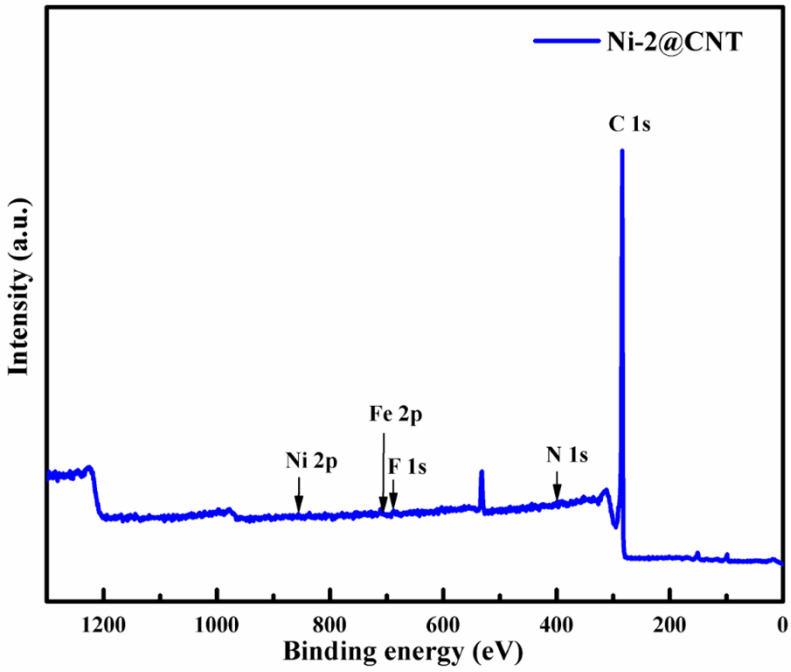

Fig. S14. XPS scan spectrum of **Ni-2@**CNT.

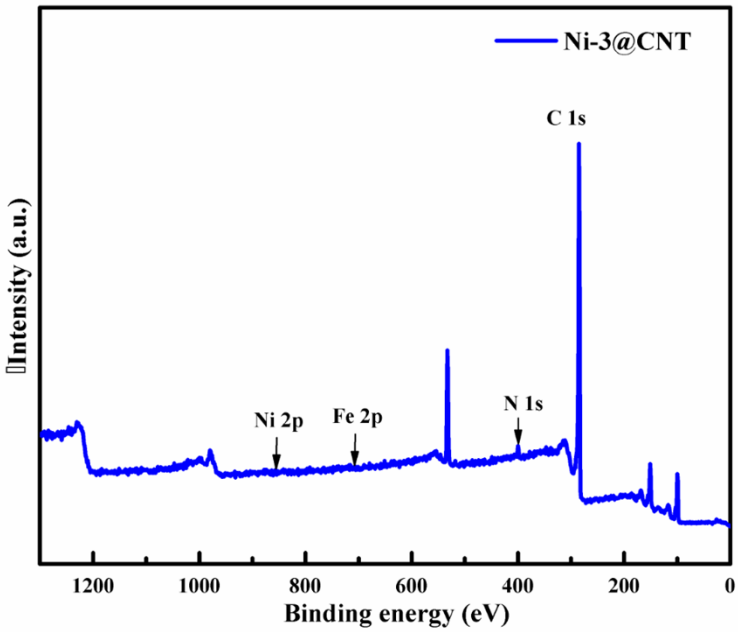

Fig. S15. XPS scan spectrum of **Ni-3@**CNT.

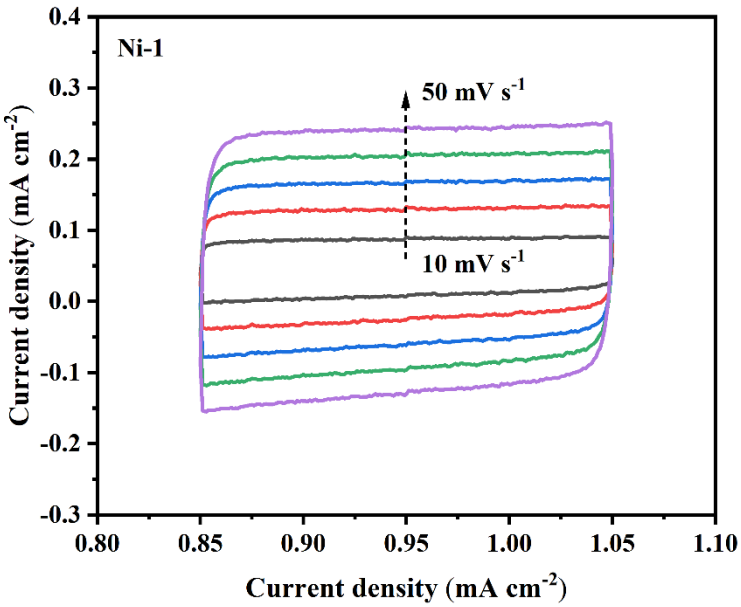

Fig. S16. CV curves of **Ni-1** at different scan rate (10-50 mV s^{-1}).

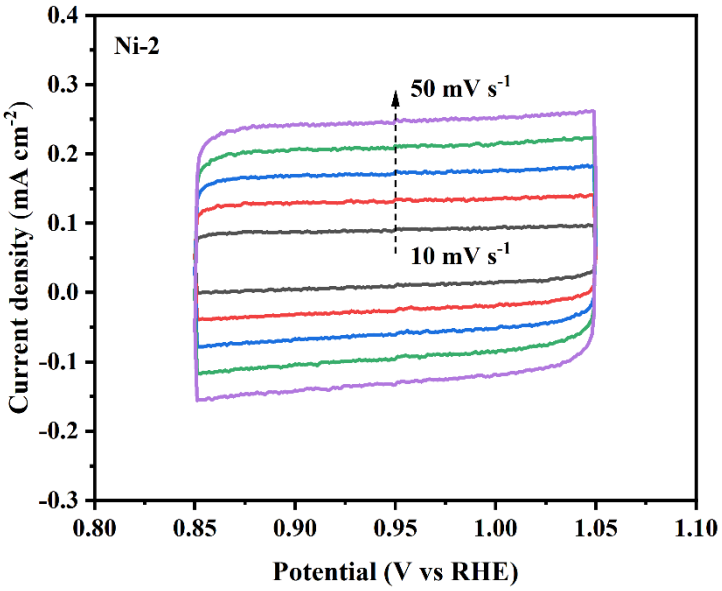

Fig. S17. CV curves of **Ni-2** at different scan rate (10-50 mV s^{-1}).

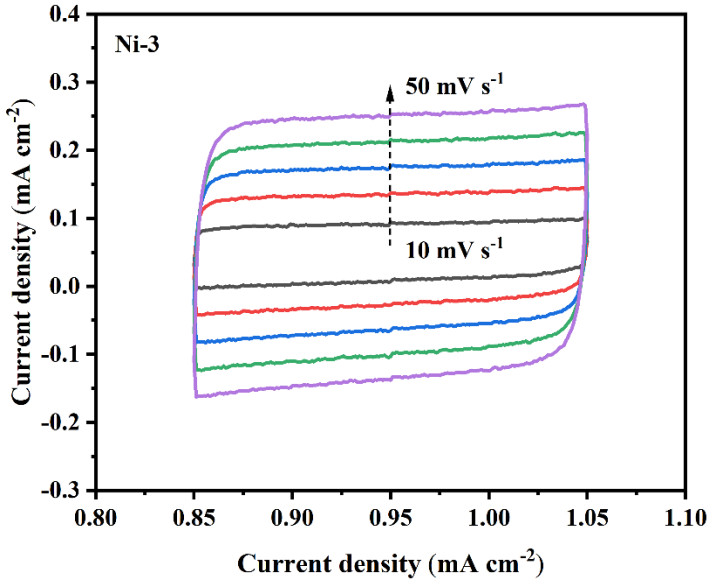

Fig. S18. CV curves of **Ni-3** at different scan rate (10-50 mV s^{-1}).

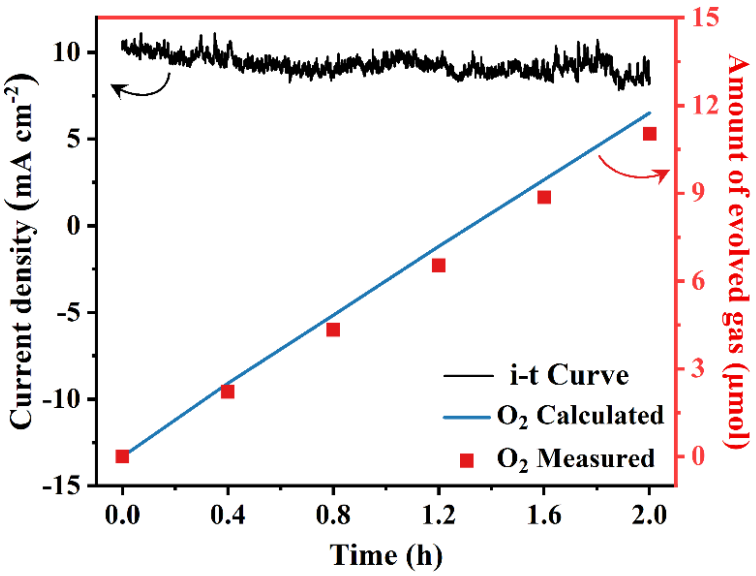

Fig. S19. The Faraday efficiency (FE) of the **Ni-3.**

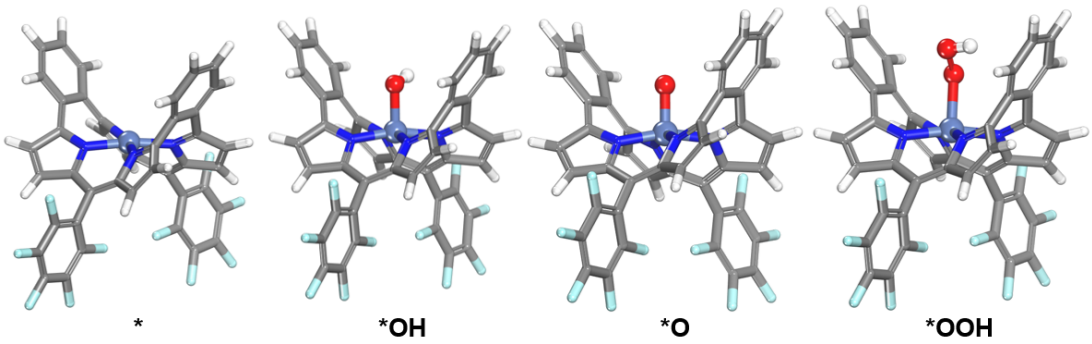

Fig. S20. DFT-optimized configurations of the intermediates (OH*, O* and OOH*) adsorbed on the surface of **Ni-1** and the catalytic path of the OER process.

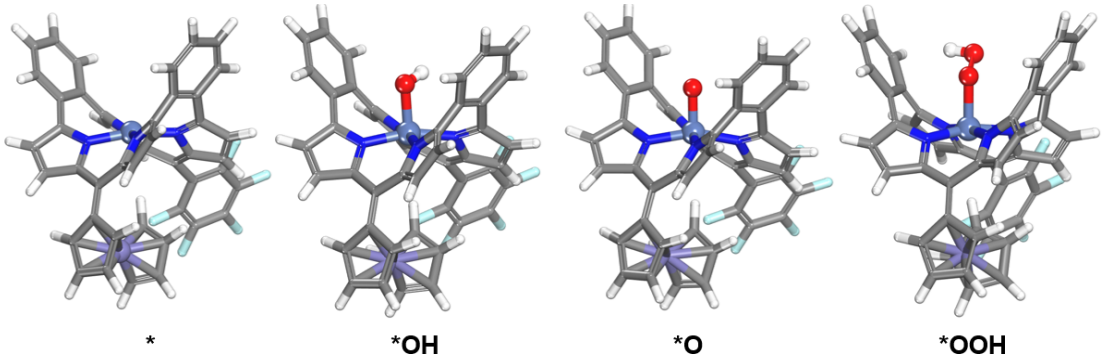

Fig. S21. DFT-optimized configurations of the intermediates (OH*, O* and OOH*) adsorbed on the surface of **Ni-2** and the catalytic path of the OER process.

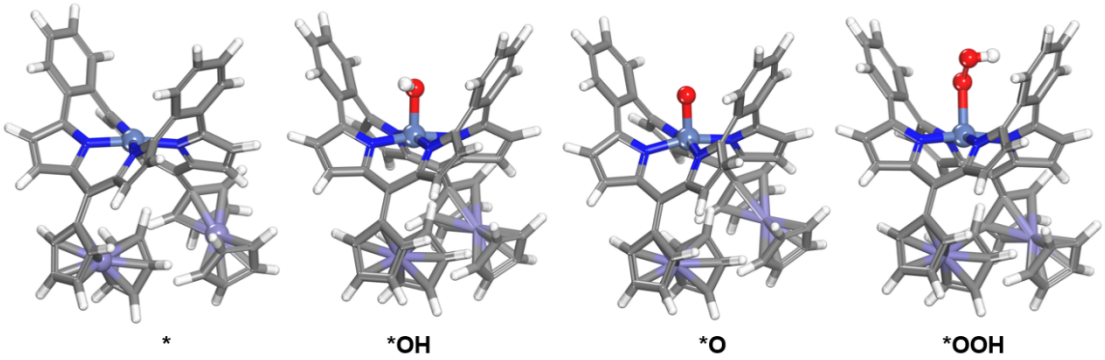

Fig. S22. DFT-optimized configurations of the intermediates (OH*, O* and OOH*) adsorbed on the surface of **Ni-3** and the catalytic path of the OER process.

3, Crystal Data.

Table S1. Crystal data of **Ni-3**

Empirical formula	$C_{50}H_{34}Fe_2N_4Ni$
Formula weight	861.22
Temperature/K	99.98(13)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	11.5014(3)
b/Å	25.4039(6)
c/Å	13.9123(4)
α/°	90
β/°	105.602(3)
γ/°	90
Volume/Å^3	3915.12(19)
Z	4
ρ_{calc}g/cm^3	1.461
μ/mm ^{1}	6.871
F(000)	1768.0
Crystal size/mm^3	0.16×0.12×0.1
Radiation	micro-focus metaljet (λ = 1.3405)
2Θ range for data collection/°	6.05 to 105.842
Index ranges	-12≤h≤13, -30≤k≤30, -16≤l≤16
Reflections collected	34824
Independent reflections	6898 [R_{int} = 0.1208, R_{sigma} = 0.0887]
Data/restraints/parameters	6898/0/514
Goodness-of-fit on F^2	1.004
Final R indexes [I>=2σ (I)]	R_1 = 0.0564, wR_2 = 0.1287
Final R indexes [all data]	R_1 = 0.0844, wR_2 = 0.1403
Largest diff. peak/hole / e Å^{-3}	0.92/-0.36

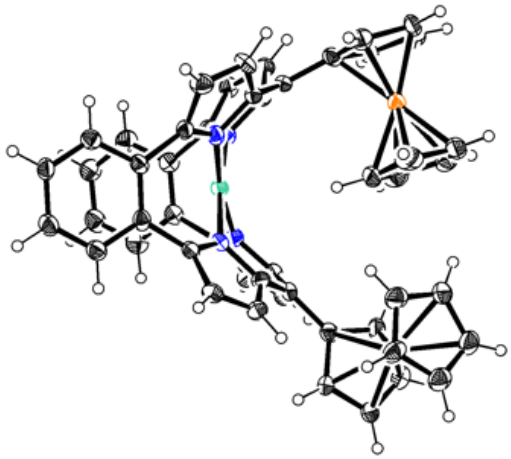

Fig. S23. Crystal structure of **Ni-3**. The thermal ellipsoids represent for 40% probability.

4, Cartesian Coordinates

Ni-1-OH

F	8.997400	6.833200	10.252600
F	7.832200	4.668200	11.418400
F	6.251600	5.001000	13.666000
F	5.918000	7.499400	14.748000
F	7.083400	9.663800	13.581400
F	11.167601	6.832800	7.666200
F	12.418600	4.670400	6.581200
F	13.999200	4.998200	4.332600
F	14.160200	7.417800	3.093000
F	12.834801	9.584200	4.165800
N	10.326400	11.115600	10.684200
N	8.083800	11.024199	9.251600
N	9.523800	10.981800	6.988800
N	11.762800	11.150399	8.415200
C	8.240400	7.013600	11.359800
C	7.650200	5.894000	11.952600
C	6.855000	6.062400	13.094400
C	6.681200	7.338200	13.645000
C	7.283401	8.442801	13.032800
C	8.051600	8.306800	11.868800
C	8.560800	9.470200	11.088800
C	9.783600	10.061600	11.421800
C	10.472000	9.967200	12.670401
C	11.368600	11.019401	12.707000
C	11.269600	11.703800	11.454801
C	12.062000	12.871400	11.065800
C	12.149800	13.957200	11.953200
C	12.953000	15.059600	11.659401
C	13.709001	15.075800	10.482599

C	13.652400	13.990999	9.606400
C	12.820601	12.890000	9.874000
C	7.707600	9.987600	10.103800
C	6.292600	9.805000	10.011999
C	5.822200	10.786400	9.159201
C	6.957200	11.513600	8.683800
C	11.897800	6.997600	6.542000
C	12.541400	5.882401	5.997000
C	13.323400	6.042600	4.845600
C	13.414400	7.291200	4.218000
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C	10.145000	9.922800	6.316800
C	9.456200	9.687201	5.087400
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C	7.446400	13.555799	5.538600
C	6.561200	14.609800	5.766800
C	5.833800	14.661200	6.960600
C	5.994000	13.656000	7.915000
C	6.902200	12.603800	7.709000
C	12.217999	10.090600	7.625400
C	13.639400	10.010400	7.737600
C	14.035601	11.065201	8.540200
C	12.852000	11.740200	8.967401
H	10.257799	9.241799	13.446799
H	12.048599	11.290600	13.505600
H	11.562000	13.934000	12.868600
H	12.990600	15.901199	12.347601
H	14.341801	15.929001	10.248600
H	14.242400	13.992000	8.692200
H	5.719400	9.072000	10.567200
H	4.798600	10.979400	8.861400
H	9.721200	8.928200	4.360600
H	7.769200	10.815600	4.185000
H	8.012800	13.505401	4.611000
H	6.437600	15.386400	5.015000
H	5.140800	15.478801	7.146200
H	5.426200	13.683400	8.842800
H	14.264999	9.288000	7.227000
H	15.041400	11.340800	8.833800
Ni	9.916200	11.334400	8.830600
H	10.395599	13.600800	8.012000
O	9.832000	13.316601	8.753000

Ni-1-O

F	9.084000	6.832200	10.329000

F	7.837400	4.664800	11.496400
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F	5.917000	7.500800	14.750400
F	7.082400	9.669600	13.582800
F	11.085200	6.831600	7.583800
F	12.498400	4.669200	6.582600
F	14.003201	4.994000	4.330000
F	14.167200	7.416600	3.084000
F	12.916201	9.584000	4.166400
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N	9.497400	10.920200	6.926600
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C	6.694200	7.349800	13.658600
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C	8.574400	9.470800	11.078000
C	9.810200	10.052200	11.375199
C	10.521000	9.971601	12.612800
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C	13.662200	15.101800	10.337200
C	13.589000	14.026600	9.452400
C	12.787000	12.907800	9.741000
C	7.717200	9.986600	10.093599
C	6.300000	9.819400	10.013400
C	5.831000	10.793400	9.149800
C	6.967800	11.502600	8.656000
C	11.864800	6.980600	6.491000
C	12.552400	5.876600	5.982600
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C	11.983800	8.249800	5.908800
C	11.387000	9.414200	6.612400
C	10.117399	9.873000	6.251600
C	9.430000	9.651200	5.016800
C	8.455000	10.628200	4.927600
C	8.509800	11.393800	6.135201
C	7.656400	12.534400	6.469000
C	7.480800	13.550800	5.512000
C	6.627400	14.625200	5.757200
C	5.913800	14.688000	6.960000
C	6.056000	13.673400	7.905400

C	6.931200	12.595400	7.681800
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C	14.020200	11.082200	8.416000
C	12.833000	11.748400	8.848800
H	10.318201	9.255600	13.400801
H	12.114201	11.301600	13.405200
H	11.615000	13.910800	12.786600
H	13.008200	15.895400	12.240601
H	14.274200	15.966600	10.090400
H	14.145201	14.045000	8.517600
H	5.724200	9.101200	10.585001
H	4.806400	10.991600	8.858800
H	9.694000	8.899200	4.282200
H	7.750000	10.796800	4.122200
H	8.038200	13.493000	4.579400
H	6.518400	15.411400	5.013200
H	5.247800	15.524799	7.159000
H	5.499400	13.710001	8.839399
H	14.255400	9.283000	7.135000
H	15.026400	11.377800	8.688200
Ni	9.915401	11.330600	8.752400
O	9.910000	13.183800	8.589600

Ni-1-OOH

F	9.000000	6.834200	10.249800
F	7.833200	4.671200	11.419000
F	6.329200	4.994800	13.671200
F	5.920000	7.498800	14.746400
F	7.083800	9.665800	13.582200
F	11.086201	6.831200	7.584400
F	12.498400	4.668600	6.582800
F	14.003000	4.994200	4.330000
F	14.166401	7.416800	3.085000
F	12.916599	9.584400	4.167200
N	10.311399	11.157200	10.672999
N	8.078600	11.006201	9.251600
N	9.499400	10.890200	6.992200
N	11.749200	11.093000	8.415000
C	8.264000	7.020600	11.365800
C	7.676600	5.901200	11.955600
C	6.898000	6.069600	13.104000
C	6.704200	7.340800	13.655400
C	7.306200	8.445200	13.044800
C	8.084400	8.312200	11.886600
C	8.580000	9.482400	11.107201
C	9.795000	10.102000	11.431800
C	10.501800	10.032801	12.669600
C	11.390200	11.096200	12.679800

C	11.263200	11.760000	11.422400
C	12.008600	12.941000	10.979000
C	12.037601	14.084600	11.798600
C	12.770000	15.213799	11.428200
C	13.500200	15.207200	10.233999
C	13.493200	14.073200	9.420600
C	12.746400	12.933599	9.772600
C	7.716800	9.977600	10.123000
C	6.304600	9.767400	10.037600
C	5.816800	10.724200	9.169399
C	6.940000	11.459599	8.676200
C	11.884399	6.985000	6.506000
C	12.563400	5.879400	5.990800
C	13.339601	6.043600	4.839200
C	13.433000	7.287000	4.211000
C	12.780200	8.386000	4.773600
C	12.017200	8.259800	5.939000
C	11.419400	9.412001	6.666400
C	10.144200	9.855600	6.313600
C	9.474000	9.617001	5.072400
C	8.481400	10.571400	4.975600
C	8.507999	11.338000	6.185000
C	7.608400	12.454600	6.477200
C	7.405200	13.434600	5.489200
C	6.512200	14.486000	5.695600
C	5.780800	14.556399	6.886200
C	5.945800	13.570600	7.859200
C	6.863800	12.522600	7.675200
C	12.226200	10.055799	7.618400
C	13.653001	10.030600	7.697400
C	14.024800	11.110000	8.481000
C	12.823400	11.741600	8.922600
H	10.307799	9.316000	13.459001
H	12.075200	11.385799	13.467600
H	11.462999	14.080200	12.723000
H	12.768200	16.095200	12.066000
H	14.071400	16.083799	9.935600
H	14.055000	14.061199	8.488800
H	5.745200	9.034800	10.606600
H	4.789400	10.896601	8.871600
H	9.761600	8.871400	4.340800
H	7.781000	10.728600	4.164000
H	7.976400	13.373600	4.565400
H	6.387000	15.247999	4.929400
H	5.083000	15.373600	7.054800
H	5.375200	13.610400	8.784801
H	14.296599	9.330400	7.178600
H	15.025400	11.431000	8.744400
Ni	9.910400	11.253400	8.823999
H	10.439000	14.614600	9.366199

O	9.919800	13.334599	8.097600
O	9.584000	14.409400	8.924800

Ni-2-OH

Ni	9.582600	11.339600	8.662600
Fe	9.918000	6.497600	6.917800
N	7.775400	11.177999	9.262000
N	10.175200	11.168200	10.458401
N	9.004200	11.155000	6.854200
N	11.332600	10.981999	8.010201
C	9.445400	10.126801	6.032200
C	7.415600	10.172400	10.167000
C	10.581200	9.329400	6.349401
C	6.632200	11.661201	8.717000
C	8.105400	11.896200	6.153400
C	7.310000	12.999801	6.684000
C	11.588800	9.898600	7.175600
C	11.227400	11.756001	11.083601
C	8.284599	9.765200	11.193800
C	12.524000	11.519600	8.382000
C	11.724800	7.007200	6.155800
C	7.158400	14.169001	5.917800
C	10.720000	7.992200	5.788000
C	11.335200	11.249800	12.417200
C	6.559000	12.856600	7.872400
C	10.074600	5.899600	4.958800
C	13.579201	10.791201	7.769200
C	6.296600	15.187799	6.322600
C	12.701000	12.683400	9.248800
C	10.321799	10.329800	12.591600
C	9.685000	7.270400	5.062600
C	11.328600	5.736800	5.632400
C	6.005400	9.957800	10.070400
C	9.568600	10.308599	11.375400
C	12.098200	12.788600	10.523601
C	13.595000	13.686800	8.833200
C	13.001400	9.754600	7.048600
C	9.234799	7.334000	8.671400
C	8.786800	10.239400	4.774200
C	7.980200	11.368400	4.841400
C	13.878599	14.786000	9.643200
C	5.671800	13.879600	8.254800
C	5.514600	10.913000	9.199800
C	5.545200	15.042200	7.493800
C	13.286800	14.888000	10.906600
C	12.415800	13.890400	11.342000
C	9.667000	5.077800	8.373400
C	10.175000	6.291400	8.947600
C	8.148600	6.779000	7.919200

C	8.413800	5.378200	7.737200
C	6.675600	9.243200	13.081400
C	6.237000	8.440600	14.135799
C	6.925400	7.269400	14.456000
C	8.019401	6.886800	13.683000
C	8.427000	7.681000	12.612400
C	7.772799	8.884000	12.276800
H	12.599000	7.188400	6.767000
H	7.742800	14.272600	5.006200
H	12.100400	11.542200	13.126201
H	9.496400	5.112200	4.488400
H	14.632799	11.020599	7.873200
H	6.209200	16.092201	5.724200
H	10.087800	9.761600	13.483400
H	8.753000	7.687000	4.704800
H	11.865999	4.804200	5.762600
H	5.441000	9.223400	10.631200
H	14.047800	13.601800	7.847800
H	13.509600	9.048400	6.405200
H	9.354400	8.379400	8.937600
H	8.979799	9.626200	3.903400
H	7.340800	11.775800	4.067600
H	14.557000	15.559200	9.289200
H	5.097000	13.758400	9.171000
H	4.484800	11.087199	8.911799
H	4.867400	15.829801	7.815000
H	13.500600	15.739799	11.548000
H	11.949000	13.965200	12.321800
H	10.155801	4.110000	8.392000
H	11.111799	6.409200	9.480400
H	7.294400	7.330800	7.542200
H	7.791600	4.675800	7.194000
F	6.006000	10.410800	12.915000
F	5.162400	8.832800	14.841000
F	6.577600	6.500000	15.501800
F	8.669001	5.749400	13.998800
F	9.499800	7.251400	11.914400
H	9.165800	13.687400	9.275400
O	9.746800	13.323400	8.584400

Ni-2-O

Ni	9.582200	11.412801	8.662800
Fe	9.917601	6.498600	6.918000
N	7.769400	11.188999	9.256200
N	10.160800	11.174200	10.450000
N	9.005200	11.184200	6.855000
N	11.328401	10.989600	8.015600
C	9.439800	10.145000	6.042200
C	7.401800	10.183600	10.154800

C	10.571800	9.340800	6.357400
C	6.635400	11.695800	8.719400
C	8.107201	11.924000	6.152600
C	7.327000	13.035601	6.688600
C	11.582600	9.906600	7.183000
C	11.198200	11.778601	11.077400
C	8.266600	9.768600	11.181400
C	12.517200	11.532600	8.386801
C	11.718201	7.021200	6.152800
C	7.175800	14.204201	5.919000
C	10.707800	8.004200	5.793600
C	11.309800	11.272000	12.409801
C	6.583600	12.898999	7.884200
C	10.069200	5.912400	4.955400
C	13.573400	10.803400	7.778200
C	6.321200	15.227200	6.325200
C	12.670200	12.709000	9.240800
C	10.305400	10.339001	12.579201
C	9.673000	7.281000	5.068800
C	11.326800	5.752000	5.623200
C	5.987400	9.989400	10.059400
C	9.553400	10.310201	11.361600
C	12.045401	12.825800	10.506400
C	13.559199	13.718801	8.823400
C	12.995800	9.765200	7.058000
C	9.228800	7.333800	8.669400
C	8.774400	10.252000	4.786600
C	7.973800	11.385799	4.846200
C	13.818001	14.830600	9.621600
C	5.705400	13.930201	8.269000
C	5.507600	10.958400	9.198200
C	5.579600	15.089001	7.504400
C	13.199400	14.946400	10.872400
C	12.332601	13.947801	11.309400
C	9.684200	5.081000	8.379400
C	10.181000	6.302400	8.946800
C	8.147000	6.763800	7.922600
C	8.426600	5.365400	7.745200
C	6.666200	9.247400	13.080200
C	6.234000	8.441800	14.135400
C	6.923800	7.271000	14.453200
C	8.011600	6.885600	13.670599
C	8.392200	7.675800	12.584800
C	7.749400	8.886600	12.263800
H	12.593401	7.203400	6.762000
H	7.749400	14.299001	4.999400
H	12.068400	11.572599	13.122000
H	9.493400	5.125000	4.482200
H	14.627000	11.032600	7.882200
H	6.230000	16.128401	5.722800

H	10.074800	9.767000	13.469600
H	8.737200	7.694201	4.717600
H	11.870001	4.821800	5.745800
H	5.414600	9.258600	10.616600
H	14.032201	13.622000	7.848400
H	13.505401	9.059200	6.415000
H	9.337200	8.381200	8.931000
H	8.960401	9.630200	3.920600
H	7.334200	11.789000	4.070600
H	14.496401	15.605000	9.270000
H	5.136800	13.815599	9.189600
H	4.479800	11.146200	8.911400
H	4.908800	15.881600	7.828200
H	13.391400	15.812000	11.502800
H	11.846400	14.032600	12.279000
H	10.182800	4.118400	8.402000
H	11.117600	6.432400	9.477200
H	7.285800	7.304800	7.545600
H	7.809800	4.654000	7.207400
F	6.002800	10.414800	12.915601
F	5.161200	8.833200	14.842200
F	6.578600	6.501000	15.500999
F	8.668200	5.751800	13.996201
F	9.421800	7.247800	11.831400
O	9.747200	13.264199	8.665200

Ni-2-OOH

Ni	9.577200	11.335000	8.661200
Fe	9.918800	6.499200	6.918200
N	7.764600	11.179000	9.245399
N	10.158600	11.180000	10.453400
N	9.004601	11.153200	6.846200
N	11.328600	10.999599	8.021601
C	9.469200	10.127601	6.030200
C	7.403200	10.180000	10.156401
C	10.601000	9.333800	6.364000
C	6.621400	11.656600	8.701400
C	8.094800	11.869600	6.129800
C	7.261400	12.957400	6.632600
C	11.599999	9.911200	7.198800
C	11.203400	11.772799	11.084599
C	8.266600	9.777600	11.182600
C	12.515800	11.545000	8.400000
C	11.745000	7.010000	6.201400
C	7.060200	14.091999	5.825400
C	10.749201	7.994800	5.808600
C	11.313200	11.271200	12.416400
C	6.523800	12.829600	7.830600
C	10.125999	5.900000	4.965000

C	13.581000	10.818400	7.807200
C	6.162400	15.091400	6.198000
C	12.654200	12.730200	9.246799
C	10.301800	10.344200	12.587000
C	9.732600	7.270600	5.058800
C	11.363000	5.738800	5.669600
C	5.990600	9.961800	10.064600
C	9.554200	10.319400	11.369200
C	12.035000	12.834999	10.515200
C	13.505000	13.766001	8.817600
C	13.013801	9.773000	7.087400
C	9.252200	7.333000	8.677999
C	8.823000	10.222401	4.763600
C	7.996200	11.334800	4.817200
C	13.724400	14.897600	9.602600
C	5.601600	13.832999	8.181800
C	5.500800	10.909801	9.191400
C	5.426600	14.961400	7.381000
C	13.103000	15.009001	10.851200
C	12.274600	13.980400	11.302800
C	9.576000	5.064000	8.340799
C	10.134400	6.239200	8.946600
C	8.151199	6.847000	7.899400
C	8.349200	5.438600	7.693000
C	6.665800	9.249800	13.079800
C	6.234800	8.441200	14.133000
C	6.923000	7.266000	14.445400
C	8.001200	6.885200	13.646601
C	8.386400	7.684400	12.572800
C	7.748800	8.895599	12.260799
H	12.603001	7.194200	6.834200
H	7.631600	14.183800	4.904200
H	12.071400	11.570400	13.130199
H	9.560400	5.112000	4.480400
H	14.632999	11.052999	7.917600
H	6.035000	15.968200	5.566401
H	10.067000	9.775400	13.478201
H	8.808200	7.683800	4.678800
H	11.898201	4.807000	5.814000
H	5.429200	9.228400	10.629801
H	13.977200	13.676800	7.841400
H	13.531400	9.063600	6.455000
H	9.420401	8.366600	8.964600
H	9.036400	9.609800	3.897800
H	7.359400	11.728400	4.034200
H	14.372200	15.692400	9.238800
H	5.038000	13.724600	9.106000
H	4.471600	11.081600	8.899401
H	4.722000	15.734400	7.679400
H	13.260799	15.889799	11.469601

H	11.792601	14.052600	12.276200
H	10.015800	4.072800	8.346600
H	11.068200	6.299000	9.494200
H	7.332000	7.448800	7.521200
H	7.700800	4.778800	7.127400
F	6.002000	10.416000	12.916000
F	5.162200	8.832600	14.841800
F	6.579800	6.501000	15.499001
F	8.668200	5.747600	13.917600
F	9.421200	7.249200	11.830400
H	10.119801	14.366799	9.947599
O	9.589000	13.420200	8.416600
O	9.250600	14.245000	9.501400

Ni-3-OH

Ni	9.751200	11.252001	9.002200
Fe	12.500600	6.159600	6.664600
Fe	7.997600	6.909200	11.082400
N	11.577600	10.757800	8.770801
N	9.491199	10.901600	7.159800
N	9.919800	11.180800	10.907801
N	7.869600	11.348000	9.262800
C	9.105400	10.374599	11.697399
C	11.970400	9.643600	8.024799
C	7.879000	9.840401	11.216400
C	12.677000	11.248600	9.394400
C	11.631001	7.954200	6.185400
C	10.841800	11.766800	11.722799
C	11.881400	12.705601	11.306000
C	12.908401	7.796000	5.521600
C	7.213600	10.505000	10.150800
C	8.698999	11.536200	6.261200
C	11.174601	9.100000	6.995000
C	6.925800	12.074600	8.601800
C	6.219400	7.874000	11.180000
C	12.089000	13.854000	12.093400
C	7.269200	8.658401	11.813601
C	8.663200	10.789200	5.046000
C	12.742200	12.461200	10.211600
C	7.095800	6.593800	12.901401
C	5.636000	11.713400	9.075400
C	13.108000	14.759800	11.800600
C	7.188800	13.078400	7.573200
C	9.452400	9.668600	5.228400
C	7.816600	7.828600	12.874001
C	6.114800	6.621400	11.858000
C	13.356000	9.404400	8.272201
C	10.010600	9.762200	6.542800
C	8.028200	12.821600	6.465400

C	6.496000	14.301600	7.638000
C	12.848200	6.621600	4.703400
C	5.808400	10.706800	10.014600
C	9.582399	7.356600	9.842200
C	9.561600	10.450601	13.044400
C	10.802200	6.846800	5.772200
C	10.620399	11.348000	13.061600
C	6.642200	15.268200	6.643400
C	13.780800	13.372001	9.943000
C	13.803200	10.427600	9.088200
C	12.778000	6.075200	8.693000
C	13.959200	14.517601	10.717800
C	7.474600	15.015000	5.548200
C	14.025600	5.891400	8.009000
C	8.149200	13.797400	5.459200
C	11.878400	5.043600	8.265400
C	11.550200	6.030800	4.862400
C	8.254000	5.464400	9.657200
C	8.509200	6.764200	9.099400
C	12.570400	4.221000	7.314800
C	13.897400	4.745400	7.153200
C	9.984200	6.439400	10.864600
C	9.166800	5.263800	10.749599
H	13.742599	8.483000	5.601600
H	5.657200	8.165600	10.302800
H	11.420799	14.037000	12.932200
H	8.102600	11.074400	4.163800
H	7.292000	5.764000	13.571000
H	4.705600	12.151400	8.734200
H	13.235001	15.650200	12.412400
H	9.689800	8.897799	4.506200
H	8.657800	8.071000	13.508600
H	5.439400	5.814600	11.596600
H	13.928200	8.590200	7.849800
H	5.850801	14.490000	8.493600
H	13.656000	6.234400	4.092200
H	5.043800	10.240601	10.622400
H	9.987600	8.353001	9.692000
H	9.088400	9.993800	13.903199
H	9.792601	6.665200	6.124200
H	11.196800	11.676800	13.918000
H	6.110200	16.213800	6.723000
H	14.436199	13.177400	9.096600
H	14.805000	10.589400	9.468000
H	12.540800	6.884400	9.374600
H	14.755800	15.217600	10.475800
H	7.598000	15.761600	4.766800
H	14.909801	6.511000	8.111400
H	8.799399	13.593201	4.611200
H	10.848400	4.932600	8.584000

H	11.208000	5.110400	4.402800
H	7.490000	4.767600	9.330200
H	7.977200	7.233600	8.278800
H	12.153999	3.371400	6.785200
H	14.659400	4.358600	6.485800
H	10.756399	6.614000	11.605600
H	9.213799	4.389000	11.388599
H	9.544600	13.629200	9.505400
O	10.082600	13.178400	8.831400

Ni-3-O

Ni	9.757600	11.496201	9.081400
Fe	12.497601	6.257000	6.670800
Fe	8.000000	6.919000	11.081800
N	11.570200	10.925400	8.853399
N	9.494400	11.071600	7.249600
N	9.916800	11.340199	10.979600
N	7.889200	11.514000	9.350600
C	9.144200	10.462399	11.734800
C	11.943600	9.782400	8.139400
C	7.923200	9.923800	11.240400
C	12.668200	11.401200	9.487200
C	11.610201	8.088600	6.291400
C	10.837999	11.910800	11.796200
C	11.850200	12.877001	11.371401
C	12.881401	7.956600	5.608200
C	7.246400	10.625000	10.202600
C	8.697800	11.702800	6.354800
C	11.153200	9.238000	7.104600
C	6.947200	12.249599	8.706800
C	6.257600	7.952600	11.160999
C	12.044400	14.032600	12.152600
C	7.323600	8.712600	11.796800
C	8.642799	10.943201	5.148600
C	12.719200	12.631399	10.281200
C	7.080800	6.659000	12.897800
C	5.658400	11.856199	9.158000
C	13.059799	14.940000	11.858601
C	7.230200	13.266200	7.695000
C	9.426800	9.819000	5.336400
C	7.841600	7.870200	12.862000
C	6.106400	6.709200	11.848600
C	13.318200	9.514600	8.420600
C	10.000000	9.917601	6.644600
C	8.052000	12.999001	6.573600
C	6.565600	14.504800	7.776400
C	12.811399	6.823800	4.734000
C	5.838800	10.817800	10.061999
C	9.595600	7.331400	9.851200

C	9.632800	10.486200	13.074800
C	10.781200	6.995200	5.843000
C	10.662001	11.417600	13.117400
C	6.714400	15.470000	6.782200
C	13.751000	13.550200	10.007800
C	13.777800	10.545000	9.223200
C	12.810000	6.079200	8.687800
C	13.918400	14.698000	10.779600
C	7.524400	15.204801	5.671600
C	14.045800	5.931200	7.973600
C	8.177200	13.978200	5.569000
C	11.904401	5.066600	8.228600
C	11.515800	6.224200	4.883400
C	8.228600	5.466000	9.659200
C	8.513800	6.760201	9.103200
C	12.580600	4.291000	7.228200
C	13.903600	4.826000	7.067400
C	9.974600	6.403600	10.873800
C	9.132200	5.245800	10.755200
H	13.715800	8.640800	5.711200
H	5.708800	8.257200	10.279200
H	11.372400	14.212600	12.989201
H	8.074400	11.220200	4.269000
H	7.244800	5.831200	13.578600
H	4.724200	12.292800	8.825800
H	13.181601	15.833200	12.467600
H	9.649400	9.038199	4.619800
H	8.684400	8.091801	13.501801
H	5.403400	5.924600	11.591999
H	13.875999	8.676400	8.024200
H	5.938200	14.701600	8.643200
H	13.609600	6.470000	4.091200
H	5.075400	10.320400	10.646600
H	10.019799	8.320200	9.704400
H	9.196800	9.971800	13.920401
H	9.776600	6.795400	6.199200
H	11.247400	11.719800	13.977600
H	6.201400	16.425001	6.872200
H	14.413800	13.352600	9.167800
H	14.776401	10.688800	9.618600
H	12.582199	6.853800	9.411600
H	14.713800	15.401000	10.541600
H	7.647600	15.951400	4.890000
H	14.929800	6.549200	8.087600
H	8.810400	13.764000	4.710600
H	10.880199	4.939200	8.560200
H	11.165400	5.328400	4.383200
H	7.452000	4.785600	9.328000
H	7.993000	7.241200	8.282000
H	12.156400	3.465200	6.667800

H	14.654599	4.472200	6.370000
H	10.746599	6.560400	11.619000
H	9.158401	4.369400	11.393400
O	10.081400	13.336000	8.916599

Ni-3-OOH

Ni	9.753000	11.334800	9.083400
Fe	12.498799	6.243600	6.666600
Fe	8.001801	6.916400	11.083401
N	11.565200	10.843400	8.816000
N	9.408600	10.938801	7.257600
N	9.987000	11.263000	10.977600
N	7.901600	11.492400	9.412800
C	9.216200	10.397000	11.752200
C	11.944400	9.728800	8.063200
C	7.960400	9.899799	11.297999
C	12.683400	11.338000	9.403200
C	11.575800	8.026600	6.240600
C	10.945601	11.792601	11.786400
C	11.949800	12.762800	11.358200
C	12.831201	7.901400	5.528800
C	7.264800	10.631400	10.301200
C	8.567600	11.532201	6.372000
C	11.120800	9.165000	7.063200
C	6.940600	12.219000	8.784000
C	6.268200	7.959400	11.196800
C	12.162400	13.910200	12.147200
C	7.345600	8.692800	11.846600
C	8.497000	10.749201	5.178800
C	12.754400	12.556800	10.213600
C	7.088600	6.614800	12.895800
C	5.661600	11.868000	9.301001
C	13.130199	14.854200	11.806001
C	7.159600	13.169800	7.697600
C	9.318200	9.654400	5.356200
C	7.859200	7.820601	12.888800
C	6.110000	6.700000	11.852799
C	13.337601	9.497601	8.269600
C	9.929000	9.795800	6.645000
C	7.903400	12.826000	6.545000
C	6.496400	14.409600	7.742800
C	12.764999	6.734800	4.700000
C	5.856200	10.847000	10.217600
C	9.572800	7.351000	9.826800
C	9.740800	10.384199	13.076000
C	10.756399	6.905000	5.847200
C	10.796000	11.287001	13.103200
C	6.573600	15.309000	6.680200
C	13.731199	13.518000	9.883400

C	13.804800	10.525399	9.070601
C	12.833200	6.137000	8.685200
C	13.915200	14.661400	10.663000
C	7.303000	14.968200	5.536000
C	14.064400	5.981000	7.964800
C	7.951400	13.735600	5.471200
C	11.937200	5.097800	8.268200
C	11.486401	6.115200	4.900200
C	8.232600	5.464200	9.660200
C	8.490200	6.760800	9.095800
C	12.614599	4.298400	7.287800
C	13.928800	4.844600	7.096600
C	9.980000	6.433800	10.847799
C	9.154800	5.261800	10.744600
H	13.652801	8.605600	5.585800
H	5.719200	8.292400	10.325600
H	11.533999	14.061001	13.022799
H	7.893600	10.997400	4.314000
H	7.249600	5.768200	13.553801
H	4.725400	12.318200	8.993800
H	13.263201	15.742001	12.420599
H	9.540200	8.869400	4.645000
H	8.705600	8.018400	13.531600
H	5.400800	5.927200	11.578799
H	13.900200	8.681800	7.837000
H	5.929399	14.663400	8.636000
H	13.557000	6.371200	4.054800
H	5.109600	10.372800	10.841800
H	9.976200	8.347600	9.671600
H	9.316600	9.865800	13.925000
H	9.766200	6.696600	6.237200
H	11.410600	11.563400	13.951599
H	6.067000	16.269600	6.743999
H	14.337999	13.356000	8.994800
H	14.815800	10.691800	9.422400
H	12.602201	6.933400	9.383801
H	14.664201	15.397201	10.378200
H	7.368400	15.659600	4.698800
H	14.942400	6.611600	8.052400
H	8.527000	13.468200	4.587600
H	10.917000	4.968600	8.611401
H	11.146000	5.192200	4.444400
H	7.462400	4.770400	9.342000
H	7.951600	7.231200	8.279799
H	12.195200	3.450400	6.757600
H	14.677800	4.477400	6.404200
H	10.759601	6.607000	11.581400
H	9.203600	4.388400	11.385401
H	11.306000	14.477201	9.359800
O	10.087399	13.408001	8.416000

O 10.327801 14.497400 9.255600

5, References

1, Hohenberg, P. & Kohn, W. Physical Review 136, B864-B871, doi:10.1103/PhysRev.136.B864 (1964).
2, Kohn, W. & Sham, L. J. Physical Review 140, A1133-A1138, doi:10.1103/PhysRev.140.A1133 (1965).
3, VandeVondele, J. et al. Comput. Phys. Commun. 167, 103-128, doi:http://dx.doi.org/10.1016/j.cpc.2004.12.014 (2005).
4, Goedecker, S., Teter, M. & Hutter, J. Phys. Rev. B 54, 1703-1710, doi:10.1103/PhysRevB.54.1703 (1996).
5, Hartwigsen, C., Goedecker, S. & Hutter, J. Phys. Rev. B 58, 3641-3662, doi:10.1103/PhysRevB.58.3641 (1998).
6, Krack, M. & Parrinello, M. Phys. Chem. Chem. Phys. 2, 2105-2112, doi:10.1039/b001167n (2000).
7, VandeVondele, J. & Hutter, J. J. Chem. Phys. 127, 114105, doi:10.1063/1.2770708 (2007).
8, Perdew, J. P., Burke, K. & Ernzerhof, M. Phys. Rev. Lett. 77, 3865 (1996).
9, Grimme, S., Antony, J., Ehrlich, S. & Krieg, H. J Chem Phys 132, 154104, doi:10.1063/1.3382344 (2010).
10, Nørskov, J. K. et al. J. Phys. Chem. B 108 (2004).
11, Rossmeisl, J., Qu, Z. W., Zhu, H., Kroes, G. J. & Nørskov, J. K. J. Electroanal. Chem. 607, 83-89, doi:10.1016/j.jelechem.2006.11.008 (2007).
12, Man, I. C. et al. ChemCatChem 3, 1159-1165, doi:10.1002/cctc.201000397 (2011).