Electronic Supplementary Information (ESI) for

A Ni (II)-based Coordination Ploymers for Efficient Electrocatalytic Oxygen Evolution Reaction

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Part I: Experimental Section

1. Ni CPs structural determination

Diffraction data of Ni (II) coordinated polymer were collected on a Bruker D8 QUEST single crystal diffractometer equipped with graphite-monochromatic Mo Kα radiation (λ = 0.71073 Å) at 273 K. The structure was solved by the direct method and refined by the SHELXTL-2014 software package. The structure determination parameters and crystallographic data are summarized in Table S1. Powder X-ray diffraction (PXRD) analyses were studied on a Rigaku Dmax2500 diffractometer with Cu Kα radiation (λ = 1.54056 Å) using a step size of 0.05°. Thermogravimetric analyses (TGA) were tested on a Mettler Toledo TGA/SDTA 851e analyzer using a heating rate of 10 °C/min under N_2 atmosphere. Elemental analyses (EA) for C, H, and N were done on an EA1110 CHNS0 CE elemental analyzer.

2. Electrochemical Measurements

All electrochemical experiments were performed in a three-electrode glass cell. The data were recorded using a CHI760 D at room temperature. The reference electrode was Ag/AgCl and the counter electrode was a platinum wire. Glassy carbon (GC, surface area = 0.196 cm^2) was acted as the substrate of working electrodes, on which the Ni based polymers were attached with 0.05 wt% nafion binder and the loading mass of sample is ~0.23 mg cm^{-2}. The linear sweep voltammetry (LSV) tests were carried out at a scan rate of 5 mV s^{-1}. The measured potentials *vs.* Ag/AgCl were converted to a reversible hydrogen electrode (RHE) scale via the Nernst equation ($E_{RHE} = E_{Ag/AgCl} + 0.059 \times pH + 0.213$). The Tafel slope was calculated according to Tafel equation ($\eta = b \cdot log(j/j_0)$).

3. Synthesis of Ni CPs

4,4'-Bipyridine (0.11g, 6.41mmol), $Ni(ClO_4)_2 \cdot 6H_2O$ (0.586g, 1.61mmol) in a water (H_2O; 5mL) solution were placed in a 23 mL vial. The sample was heated at 130 °C for two days, and then cooled to room-temperature. After washing with distilled water, the blue crystals were obtained (51% yield). EA calc. (%) for $C_{40}H_{36}Cl_2N_8NiO_{12}$: C, 50.51; H, 3.78; N, 11.79; found: C 50.57, H 3.76, N, 11.81.

3.1 Synthesis of Fe@Ni-CPs

Fresh **Ni-CPs** sample was immersed in $(NH_4)_2SO_4 \cdot FeSO_4 \cdot 6H_2O$ solution (10 mM) for 4 hours. Further, the obtained **Fe@Ni-CPs** was washed with water and ethanol three times before use.

4. Ni-CPs coated on glassy carbon electrode (Ni-CPs@GC)

The as-synthesized **Ni-CPs** was firstly dispersed in the mixture of 1 ml of 0.05 wt.% nafion water solution, and then transferred onto the glassy carbon electrode with a loading amount of ~ 0.23 mg cm^{-2}. The resulting electrode was drying in air for 4 h before use.

4.1 Fe@Ni-CPs coated on glassy carbon electrode (Fe@Ni-CPs@GC)

The procedure for preparation of **Fe@Ni-CPs@GC** is similar to **Ni-CPs@GC** except for using **Fe@ Ni-CPs** instead of **Ni-CPs**.

4.2 Ru/C coated on glassy carbon electrode (Ru/C@GC)

The procedure for preparation of **Ru/C@GC** is similar to **Ni-CPs@GC** except for using **Ru/C** in place of **Ni-CPs**.

Part II: Supplementary Results

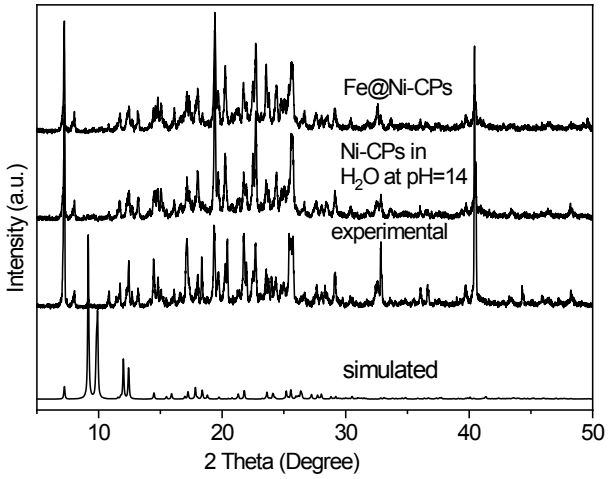

Figure S1. The PXRD patterns of Ni CPs under different conditions.

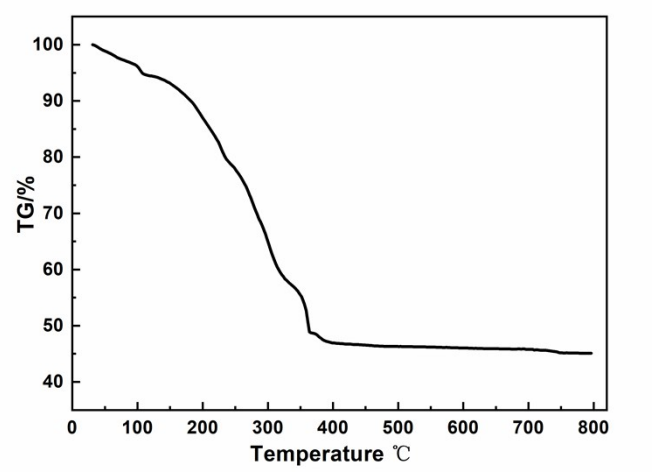

Figure S2. Thermogravimetric profiles recorded for Ni-CPs.

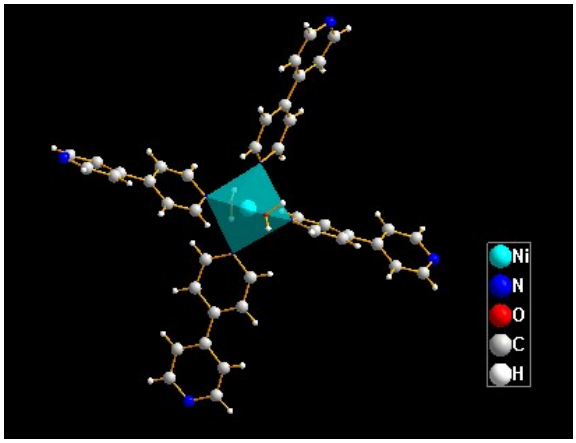

Figure S3. The coordination environment of Ni-CPs.

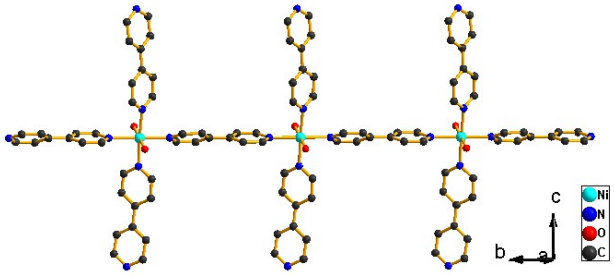

Figure S4. The single chain of Ni-CPs.

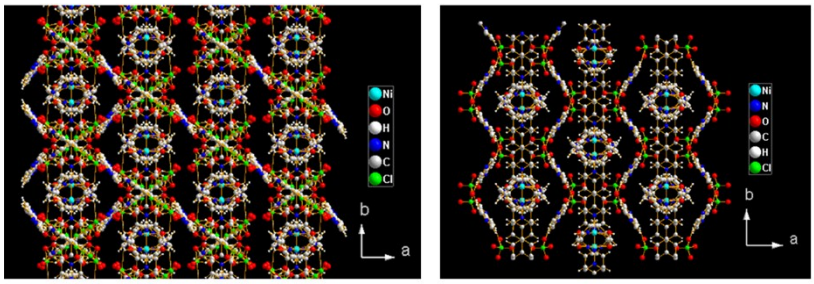

Figure S5. The 3D packing of Ni CPs（left: reported, right: this work）.

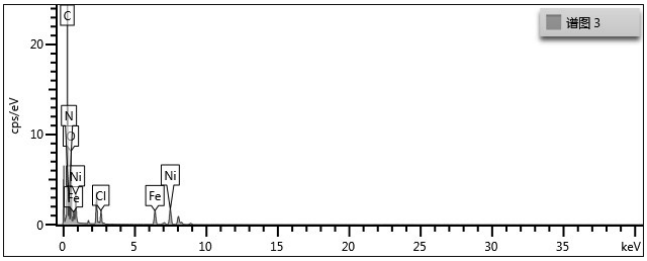

Figure S6. EDX of Fe@ Ni- CPs.

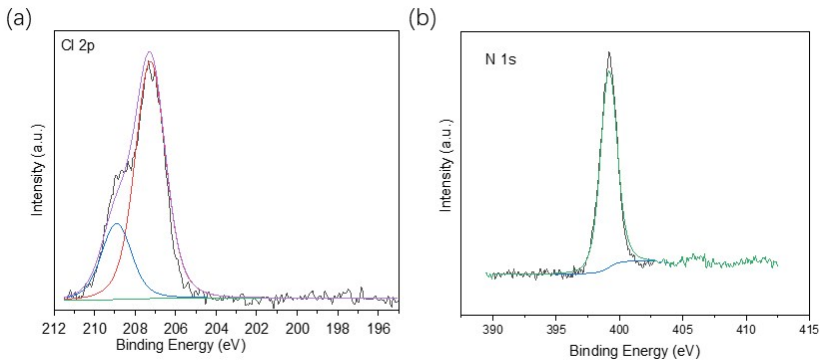

Figure S7. XPS spectrum of the Cl 2p (a) and N1s(b).

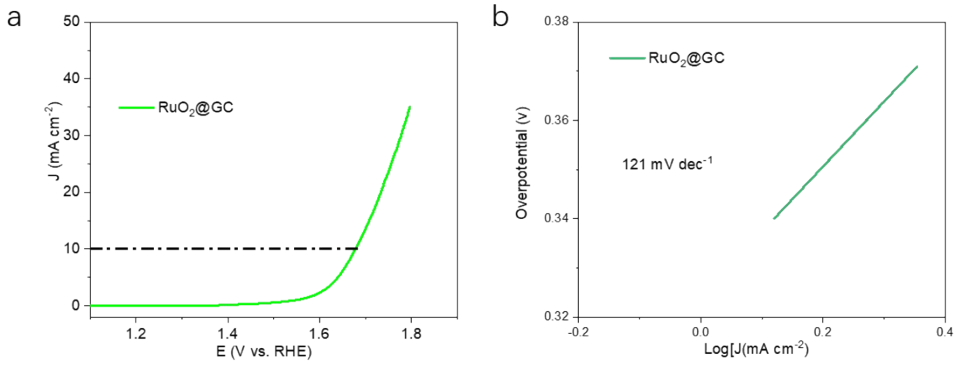

Figure S8. (a) LSV curves of RuO_2/C@GC and (b)Tafel plots of RuO_2/C at pH = 14.

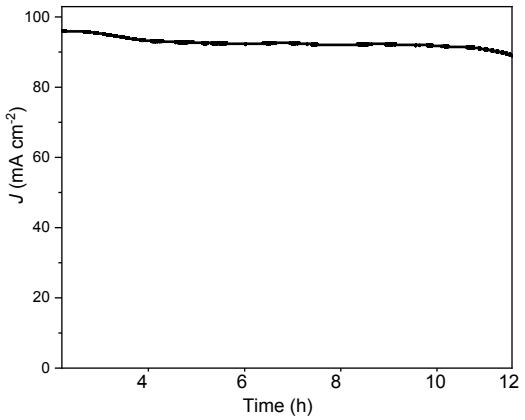

Figure S9. Chronoamperometric curves of Fe@ Ni-CPs conducted at 1.55 V.

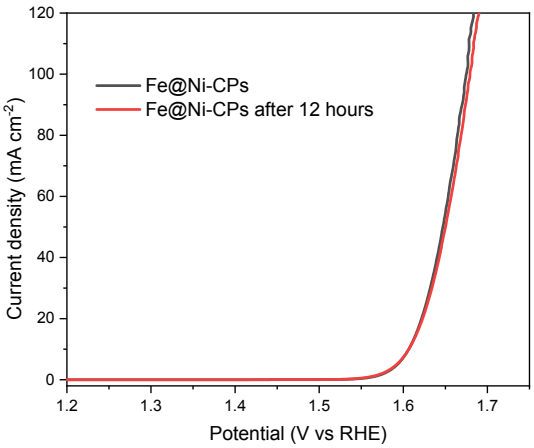

Figure S10. LSV of Fe@ Ni-CPs after 12 hours stability test in 1 M KOH aqueous solution.

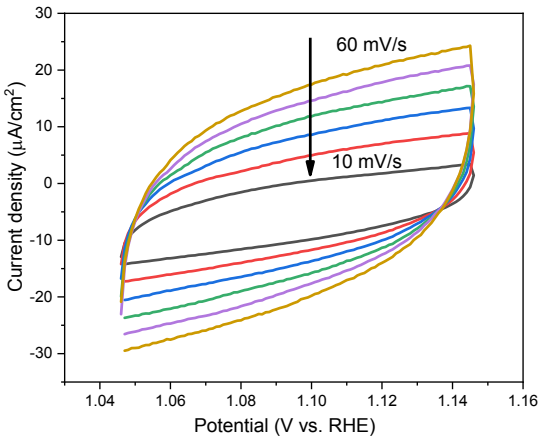

Figure S11. CV curves at different scan rates in the range of 1.04 and 1.15 V vs. RHE for Fe@ Ni-CPs.

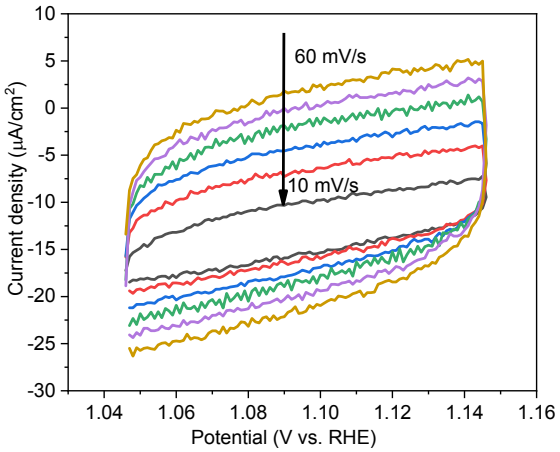

Figure S12. CV curves at different scan rates in the range of 1.04 and 1.15 V vs. RHE for Ni-CPs

Table S1. Summary of crystalographic data and refinement results.

	Ni-CPs
chemical formula	$C_{40}H_{36}Cl_2N_8NiO_{12}$
formula mass	950.36
Space group	*C2/c*
a/Å	17.9784(12)
b/Å	11.4346(8)
c/Å	24.4647(17)
α/°	90.00
β/°	92.082(2)
γ/°	90.0
Volume/Å^3	5026.0(6)
Temperature/K	273(2)
Z	4
absorption coefficient (μ/mm^{-1})	0.554
No. of reflections measured	23130
No. of independent reflections	4962
R_{int}	0.0401
GOF on F^2	0.997
R_1,[a] wR_2 [I > 2δ(I)]	R_1 = 0.1032, wR_2 = 0.3371
R_1, wR_2 (all data)	R_1 = 0.1181, wR_2 = 0.3562
CCDC Number	1858717

[a]$R_1 = \Sigma(|Fo| - |Fc|)/\Sigma|Fo|$, $wR_2 = [\Sigma w(Fo^2 - Fc^2)^2/\Sigma w(Fo^2)^2]^{0.5}$

Table S2. Comparison of the OER activities of **Fe@Ni-CPs** with reported MOF-based electrocatalysts supported on different substrates.

Catalyst	Onset potential (V vs.RHE)	Over-potential at 10 mA cm^{-2} (mV vs. RHE)	Tafel Slope (mV dec^{-1})	Substrate	Ref
MAF-X27-OH	1.47	292	88	Cu Foil	1
Co-ZIF-9	NA	510 at 1 mA cm^{-2}	193	FTO glass	*2*
Co-WOC-1	1.62	390 at 1 mA cm^{-2}	128	GC	3
USTA-16	1.60	408	77	GC	4
Co/MIL-100(Fe)	1.58	734 (5mA cm^{-2})	NA	GC-RDE	5
Ni/Fe-BTC	NA	270	43	NF	6
Co/MIL-101	1.53	477	122	GC-RDE	7
NiFe-MOF-74	NA	223	76	Ni Foam	8
MOF NU-1000	NA	320	59	FTO glass	9
CoOx-ZIF/C	1.548	318	70	Glassy carbon	10
Ni-CPs	**1.62**	**458**	**97**	**GC**	**This work**
Fe@Ni-CPs	**1.52**	**368**	**59**	**GC**	**This work**

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