Electronic Supplementary Material (ESI) for Nanoscale.

3D hollow Co-Fe-P nanoframes immobilized on N,P-doped CNT as an efficient electrocatalyst for overall water splitting

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Faradaic efficiency calculation

During the OER (or HER), n_{O_2}(experimental) (or n_{H_2}(experimental)) is estimated from the observed gas amount and the theoretical number of moles of oxygen (or hydrogen) evolved can be calculated using the following equation：

$$n_{O_2 or H_2}(\text{theoretical}) = \frac{Q}{nF}$$

Where $n_{O_2 or H_2}$ is the number of moles of oxygen (or hydrogen) produced, Q is the charge passed through the electrodes, F is the Faradaic constant (96485 C mol^{-1}), and *n* is the number of electrons transferred during OER (four moles of electrons per mole of O_2) or HER (two moles of electrons per mole of H_2). Thus, Faradaic efficiency can be determined by the following equation:

$$\text{Faradaic efficiency} = \frac{n\ (experimental)}{n\ (theortical)} \times 100\%$$

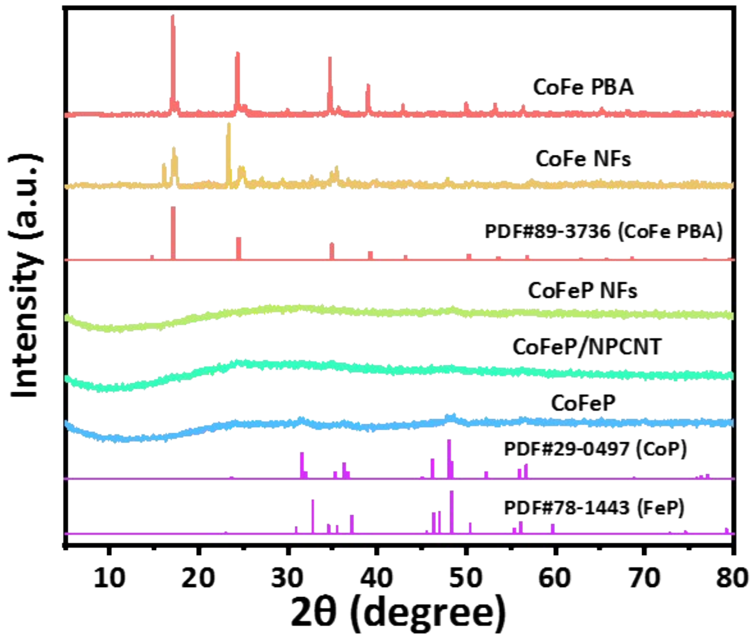

Fig. S1 XRD patterns of CoFe PBA, CoFe NFs, CoFeP NFs, CoFeP/NPCNT and CoFeP.

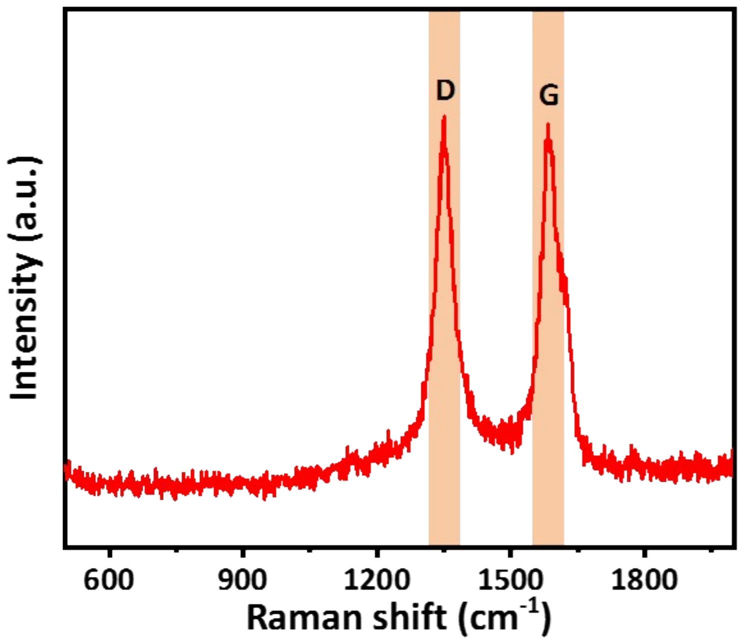

Fig. S2 Raman pattern of CoFeP NFs/NPCNT.

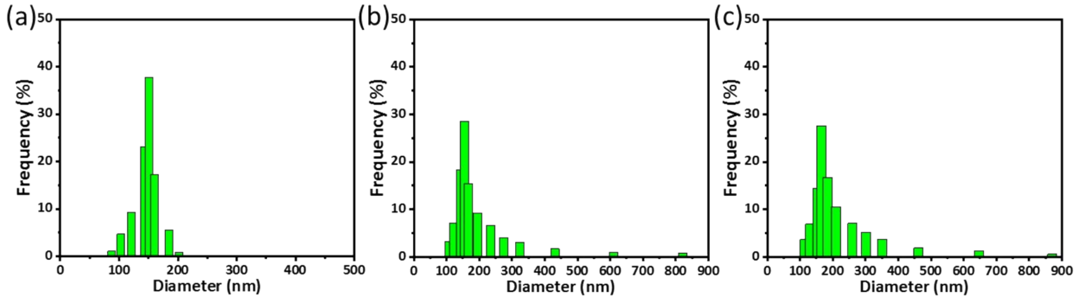

Fig. S3 Particle size distribution histograms of (a) CoFe PBA/CNT, (b) CoFe NFs/CNT and (c) CoFeP NFs/NPCNT.

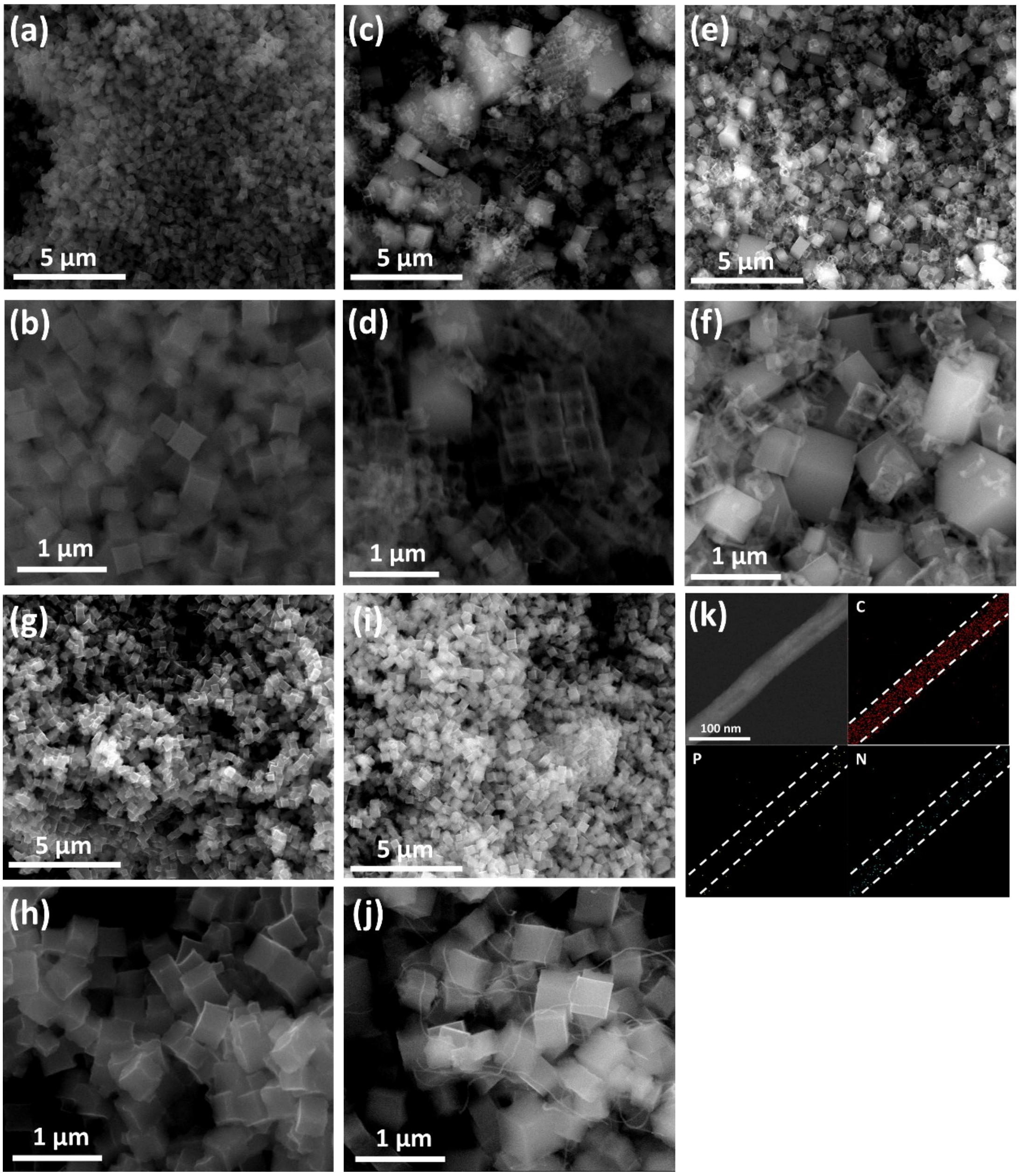

Fig. S4 The SEM images of CoFe PBA (a-b), CoFe NFs (c-d), CoFeP NFs (e-f), CoFeP (g-h) and CoFeP/NPCNT (i-j). EDS element mapping image (k) of N,P doped CNT

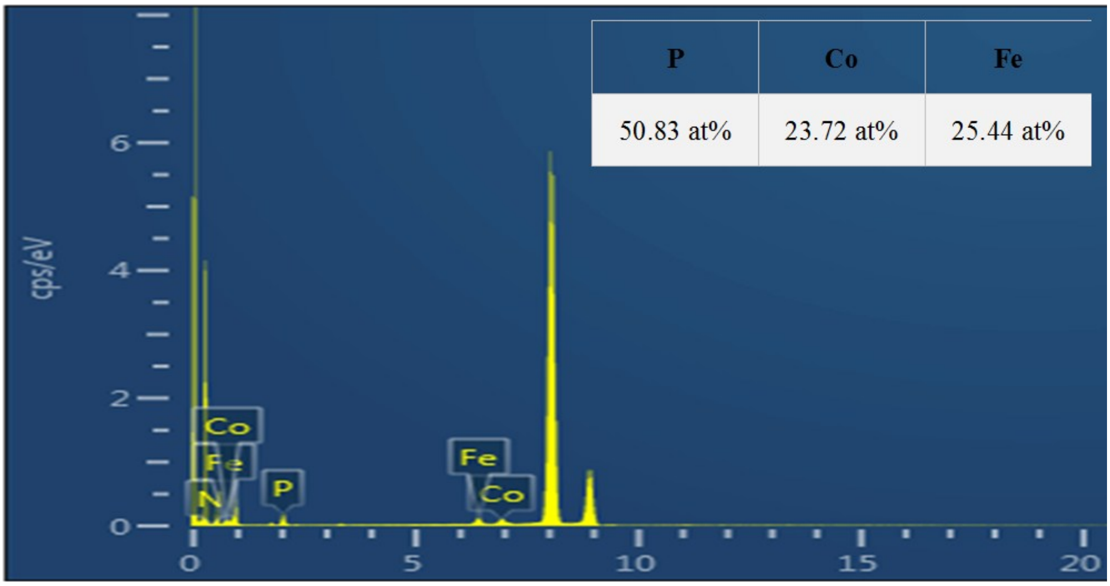

Fig. S5 EDS spectra of the CoFeP NFs@NPCNT

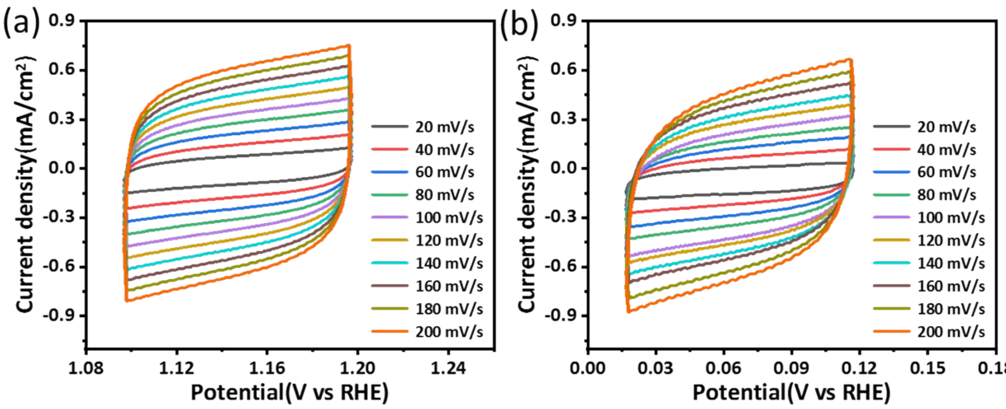

Fig. S6 (a) The cyclic voltammograms of CoFeP NFs/NPCNT in the potential range between 1.097 to 1.197 V vs RHE for OER. (b) The cyclic voltammograms of CoFeP NFs/NPCNT in the potential range between 0.017 to 0.117 V vs RHE for HER.

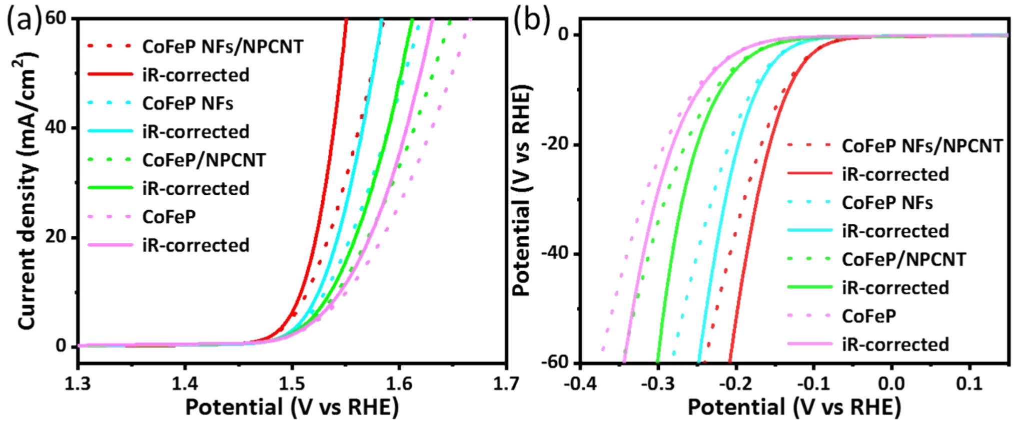

Fig. S7 (a) OER LSV curves and (b) HER LSV curves of the catalysts in 1.0 M KOH with and without iR correction.

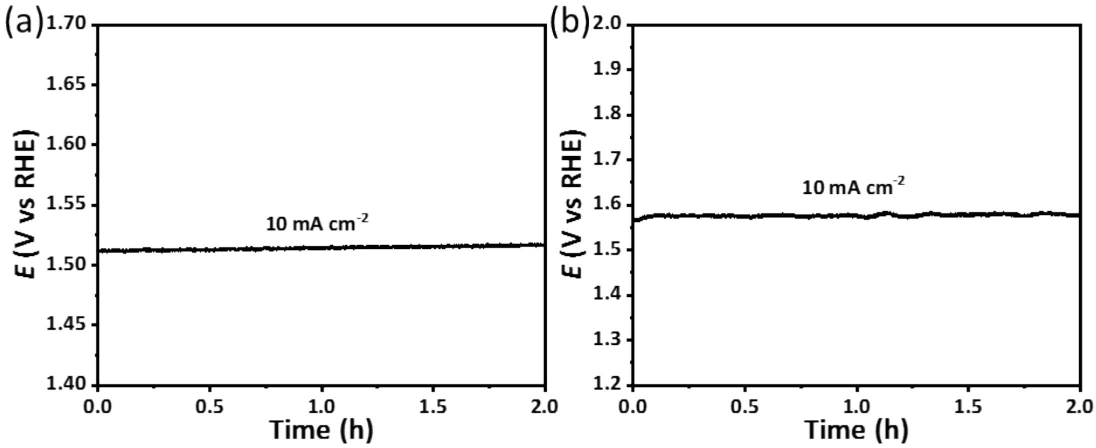

Fig. S8 Chronopotentiometric curves of the CoFeP NFs/NPCNT catalyst at 10 mA/cm^2 for (a) OER and (b) water-splitting in 1.0 M KOH.

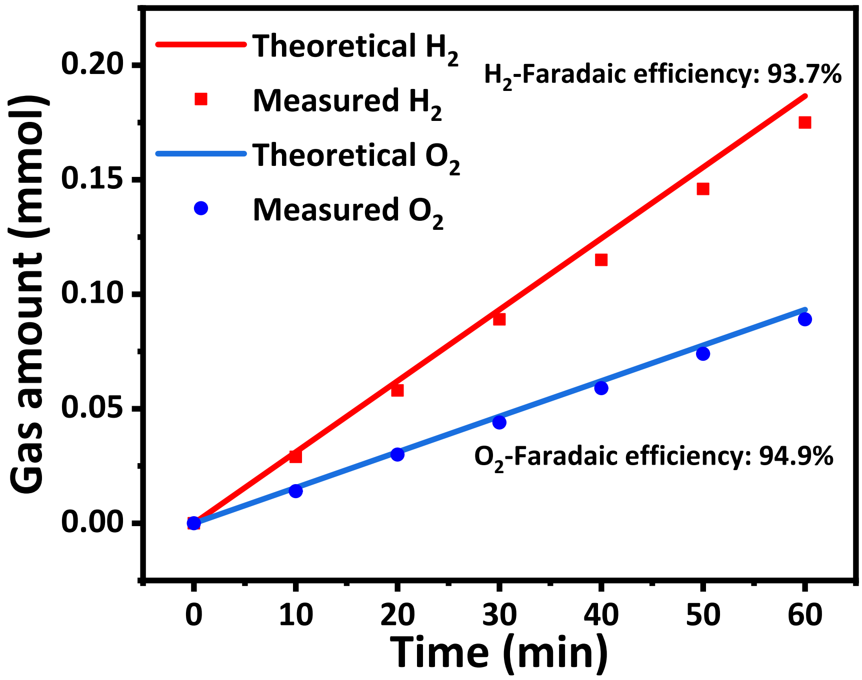

Fig. S9 The theoretical and measured yields of H_2 and O_2 over time during electrolysis of CoFeP NFs/NPCNT electrode at the current density of 10 mA cm^{-2}. Faradaic efficiency of CoFeP NFs/NPCNT electrode for H_2 and O_2 evolution in comparison with theoretical estimation

Table

Table S1 Summary of OER performance of some catalysts in previous works and our work

Samples	Tafel slope (mV/dec)	Over potential (mV) @10mA/cm^2	Electrolyte	References
CoFeP NFs/NPCNT	42.8	285	1 M KOH	This work
CoP/CoP_2 @ NPCNTs	67	300	1 M KOH	1
porous Ni_2P NS	105	320	1 M KOH	2
$Co_{0.6}Fe_{0.4}P$-1.125	48	297	1 M KOH	3
Co_2P/NPCNT	53	370	1 M KOH	4
$CoNi_{0.2}Fe_{0.05}$-Z-H-P	48.2	316	1 M KOH	5
Co_3S_4 @ MoS_2	43	280	1 M KOH	6
Co_2P/Co-Foil	79	319	1 M KOH	7
Ni_xP_y-325	72.2	320	1 M KOH	8
CoNiBO nanosheets	60	300	1 M KOH	9
NiCoFe MOF	49	320	1 M KOH	10
NiCoP/C	96	330	1 M KOH	11
Ni @ NC-800	45	280	1 M KOH	12
CNTs @ NiCoP/C	57.3	297	1 M KOH	13
NiCoP/NC PHCs	51	297	1 M KOH	14

Table S2 Summary of HER performance of some catalysts in previous works and our work

Samples	Tafel slope (mV/dec)	Over potential (mV) @10mA/cm^2	Electrolyte	References
CoFeP NFs/NPCNT	64.1	137	1 M KOH	This work
porous Ni_2P NS	63	168	1 M KOH	2
Co_3S_4 @ MoS_2	74	136	1 M KOH	6
Co_2P/Co-Foil	59	157	1 M KOH	7
Ni_xP_y-325	107.3	160	1 M KOH	8
CoNiBO nanosheets	116	140	1 M KOH	9
NiCoFe MOF	114	270	1 M KOH	10
Ni @ NC-800	160	205	1 M KOH	12
Ni_2P/CoP NP	67	184	1 M KOH	15
NiCoP/rGO	124.1	209	1 M KOH	16
NiFe LDH-NS@DG10	110	300	1 M KOH	17
NDGL coated Fe-Ni	133.2	201	1 M KOH	18
NiS/NiS_2	95.1	143	1 M KOH	19
$Ni_{1.5}Fe_{0.5}P$	125	282	1 M KOH	20
NOGB-800	98	220	1 M KOH	21

Table S3 Summary of overall water-splitting performance of some catalysts in previous works and our work

Samples	Potential (V) @10mA/cm^2	References
CoFeP NFs/NPCNT	1.56	This work
$Co_{0.6}Fe_{0.4}P$-1.125	1.57	3
Co_3S_4 @ MoS_2	1.58	6
Co_2P/Co-Foil	1.71	7
Ni_xP_y-325	1.57	8
CoNiBO nanosheets	1.69	9
Ni @ NC-800	1.6	12
NiCoP/rGO	1.59	16
NDGL coated Fe-Ni	1.701	18
NiS/NiS_2	1.62	19
NOGB-800	1.65	21
$NiCo_2P_2$/GQD nanosheet array	1.61	22
Ni-Co-P HNBs	1.62	23
Co_4Ni_1P NTs	1.59	24
(Ni,Co)Se_2-GA	1.6	25

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