Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Novel nickel-cobalt phosphite with face-sharing octahedra derived electrocatalyst for efficient water splitting

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Keywords: Cobalt-nickel microporous materials, Ni_2P, theoretical calculation, water splitting.

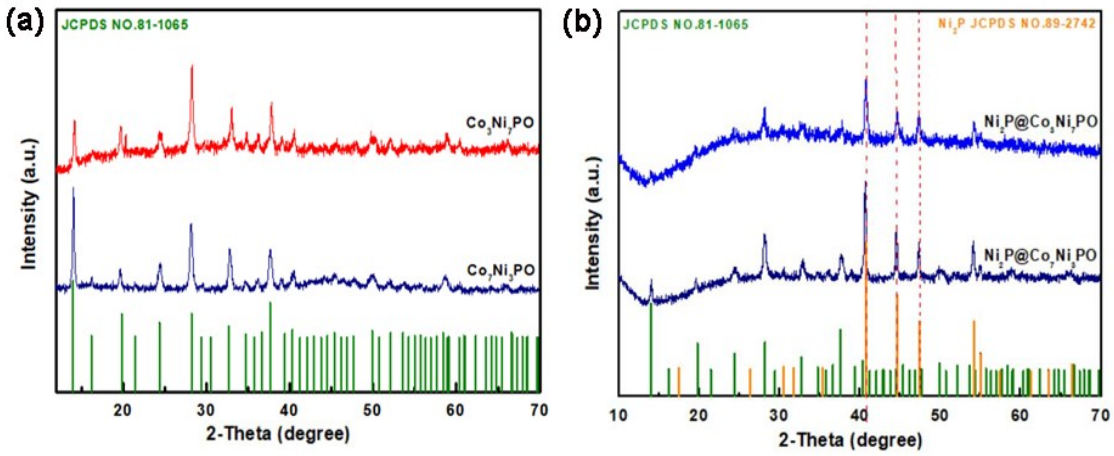

Figure S1. XRD pattern of Co_3Ni_7PO and Co_7Ni_3PO (a); $Ni_2P@Co_3Ni_7PO$ and $Ni_2P@Co_7Ni_3PO$ (b).

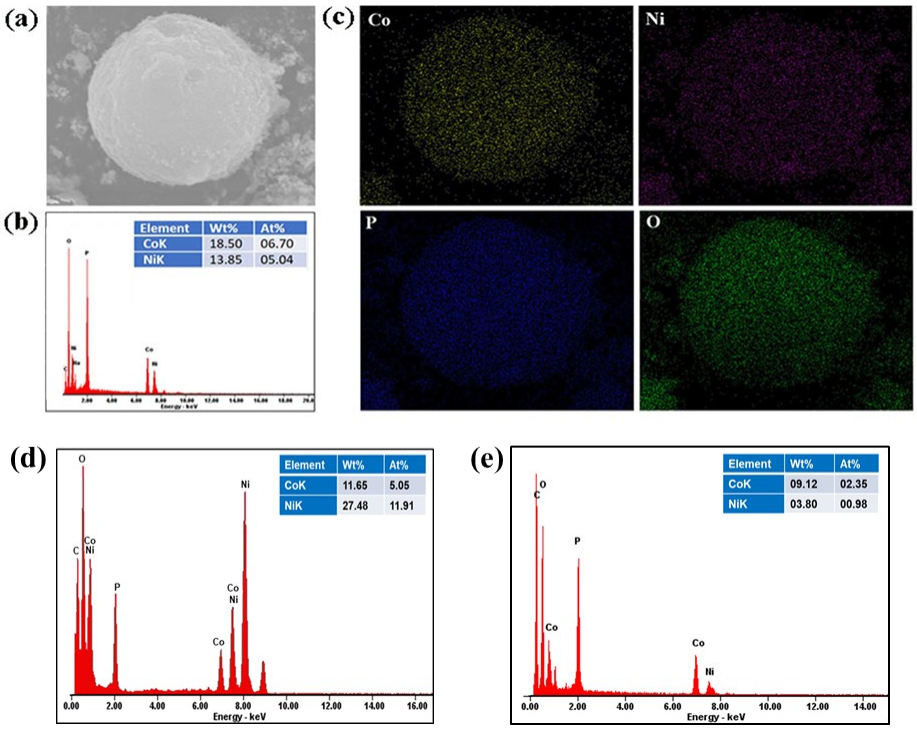

Figure S2. (a) SEM images of CoNiPO. (b) The EDS spectrum of CoNiPO. (c) Elemental mapping images of CoNiPO with yellow for Co, blue for Ni, gray for O and red for P, respectively. The EDS spectrum of Co_3Ni_7PO (d) and Co_7Ni_3PO (e).

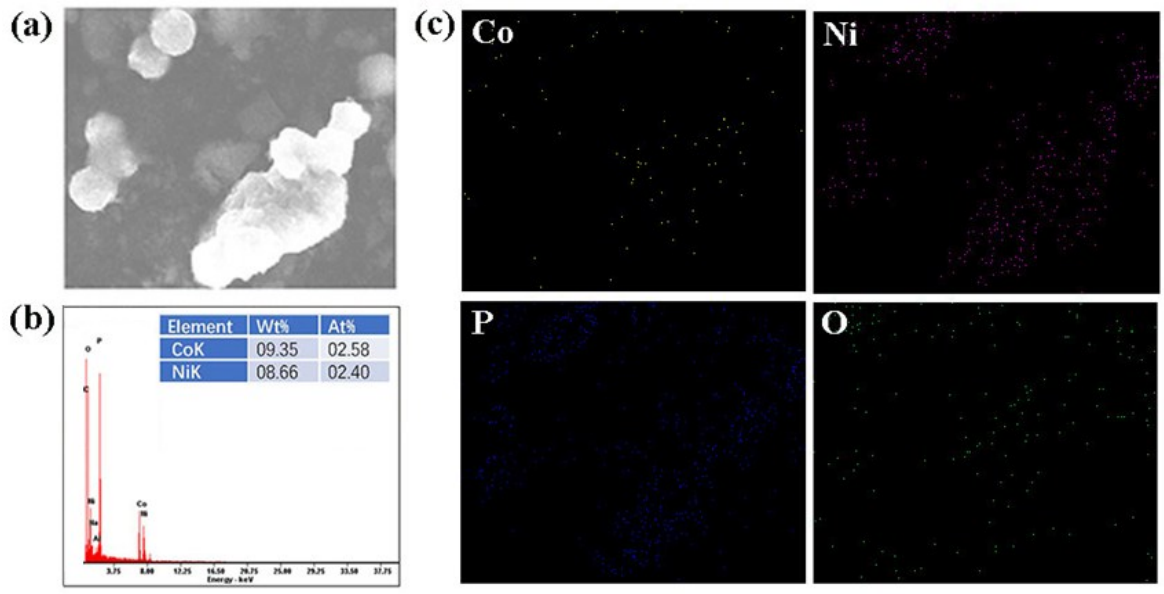

Figure S3. (a) SEM images of Ni_2P@CoNiPO. (b) The EDS spectrum of Ni_2P@CoNiPO. (c) Elemental mapping images of Ni_2P@CoNiPO with yellow for Co, blue for Ni, gray for O and red for P, respectively.

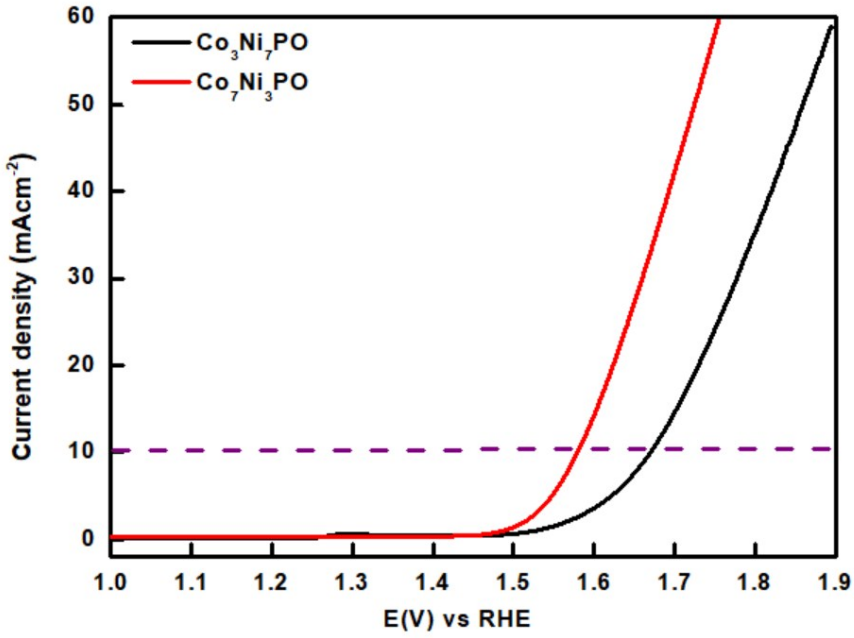

Figure S4. Polarization LSV curves of Co_3Ni_7PO and Co_7Ni_3PO.

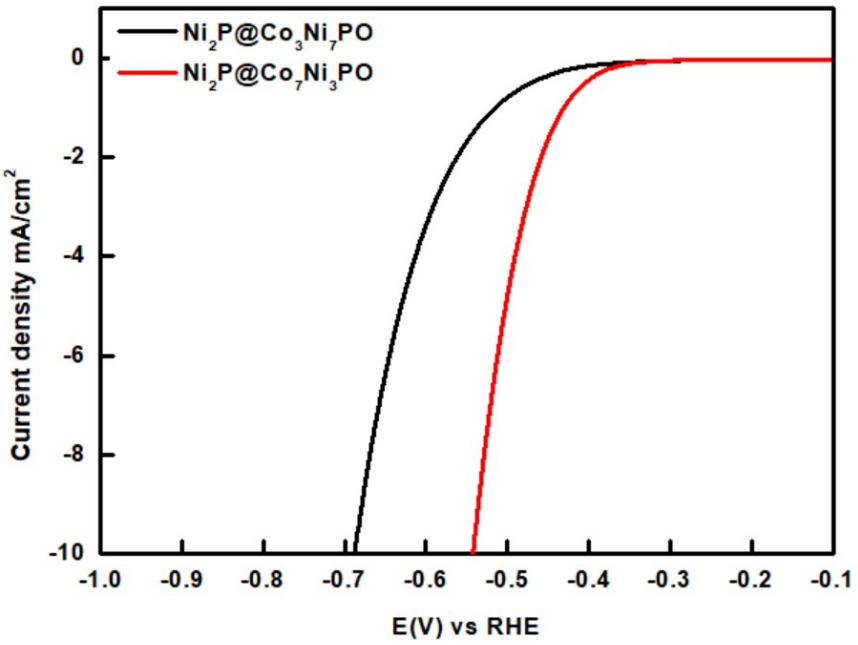

Figure S5. Polarization LSV curves of $Ni_2P@Co_3Ni_7PO$ and $Ni_2P@Co_7Ni_3PO$.

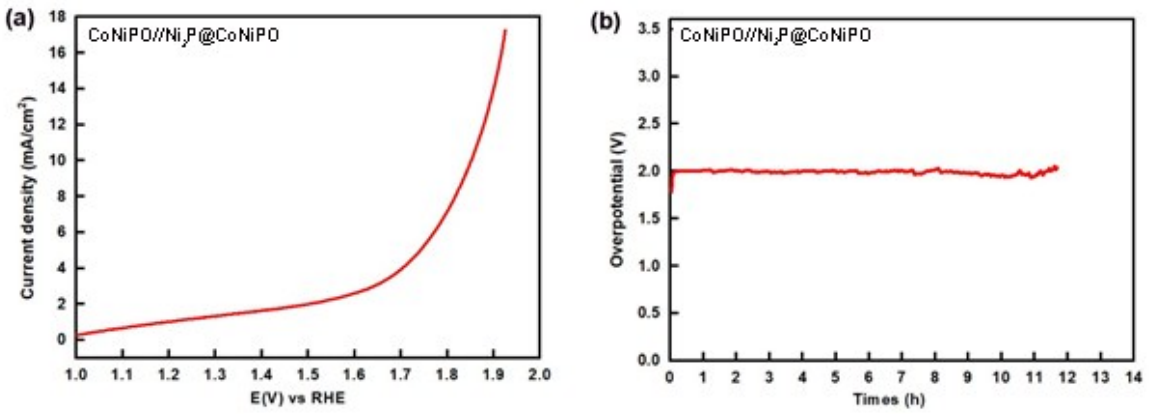

Figure S6. (a) Polarization LSV curves and (d) Time-dependent current density curve of OER at 10 mA cm^{-2} using CoNiPO//Ni_2P@CoNiPO as catalyst.

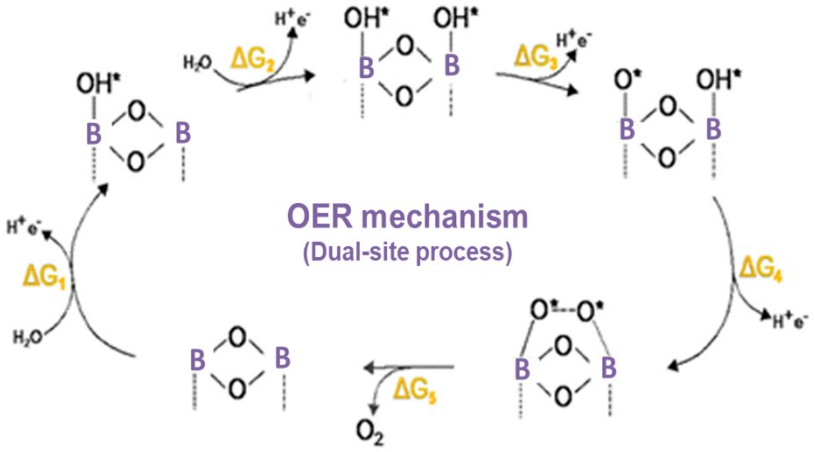

Figure S7. OER mechanism using a two-site model. After four electron-proton electrochemical steps labeled as ΔG(1-4), there is an additional pure chemical step ΔG5. [4]

Table S1. Comparison of the OER activity for several recently reported active non-metal based electrocatalysts in alkaline solution.

Electrocatalysts	Overpotetial(mV) j =10mA/cm^{-2}	Tafel slope (mV dec^{-1})	Electrolyte (pH)	Reference.
NiCoPO	320	84	0.1 M KOH	This work
NiPO	370	121	0.1 M KOH	This work
CoPO	400	139	0.1 M KOH	This work
NiOOH	360	111	0.1 M KOH	1
γ-CoOOH	300	~	0.1 M KOH	2
α-$Ni(OH)_2$ spheres	331	42	0.1 M KOH	3
β-$Ni(OH)_2$ nanoplates	444	111	0.1 M KOH	3
$LiNiO_2$	500	68	0.1 M KOH	4
NiCo-LDH	290	~	0.1 M KOH	5
Ni-Co binary oxide	325	39	0.1 M KOH	6
Ni-Co oxide nanosheets	340	51	0.1 M KOH	7

Table S2. Comparison of the HER activity for several recently reported nickel phosphides based electrocatalysts in acid solution.

Electrocatalysts	Overpotetial (mV) j =10mA/cm^{-2}	Tafel slope (mV dec^{-1})	Electrolyte (pH)	Reference.
Ni_2P@NiCoPO	180	47	0.1 M KOH	This work
Ni_2P@NiPO	400	109	0.1 M KOH	This work
Ni_2P nanoparticles	130	84	0.1 M KOH	8
Ni_2P nanorods	131	106	0.1 M KOH	9
N_2P/GC	120	87	0.1 M KOH	10
N_2P/Ni foam	120	60	0.1 M KOH	11
N_2P/Carbon	115	54	0.1 M KOH	12
Ni_2P NPs/Ti	138	60	0.1 M KOH	13
$Ni_{12}P_5$ nanopartcles	175	63	0.1 M KOH	14
Ni_5P_4-Ni_2P nanosheet	140	79.1	0.1 M KOH	15

Reference

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