Supporting Information

Multifunctional characteristics of one-dimensional bimetallic oxyhydroxide nanorods coupled polyaniline interface accelerated water and urea electrolysis

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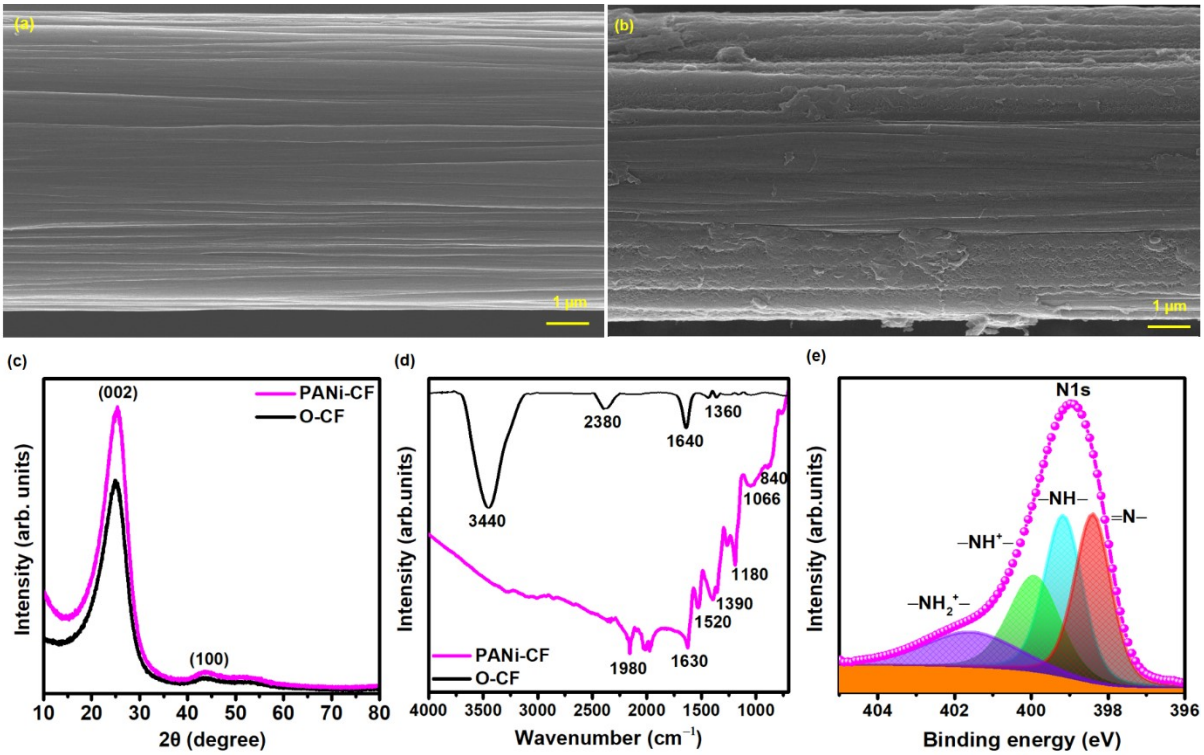

Figure S1. FESEM images of (a) O-CF and (b) PANi-CF. (c) XRD patterns and (d) FTIR spectra of O-CF and PANI-CF. (e) Deconvoluted N 1*s* XPS spectra of PANi-CF.

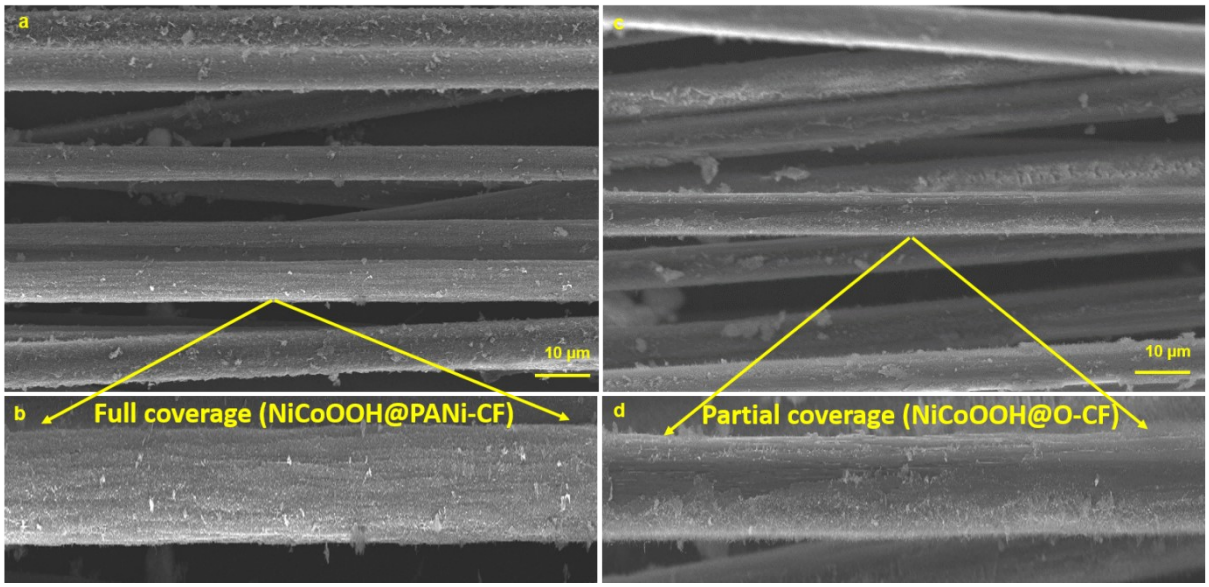

Figure S2. FESEM images of the (a and b) NiCoOOH@PANi-CF and (c and d) NiCoOOH@O-CF under different magnifications.

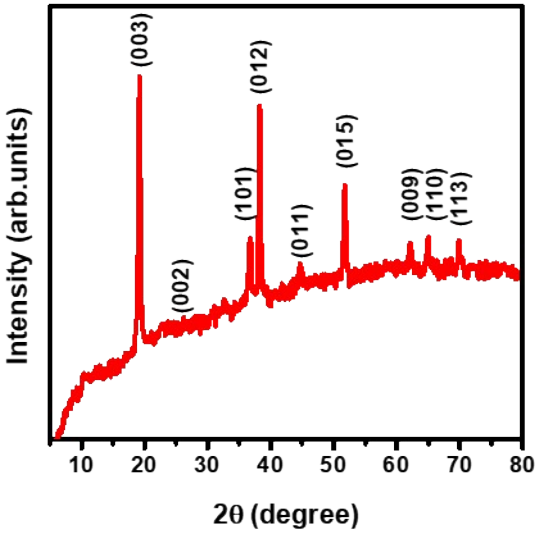

Figure S3. XRD spectrum of NiCoOOH@PANi-CF.

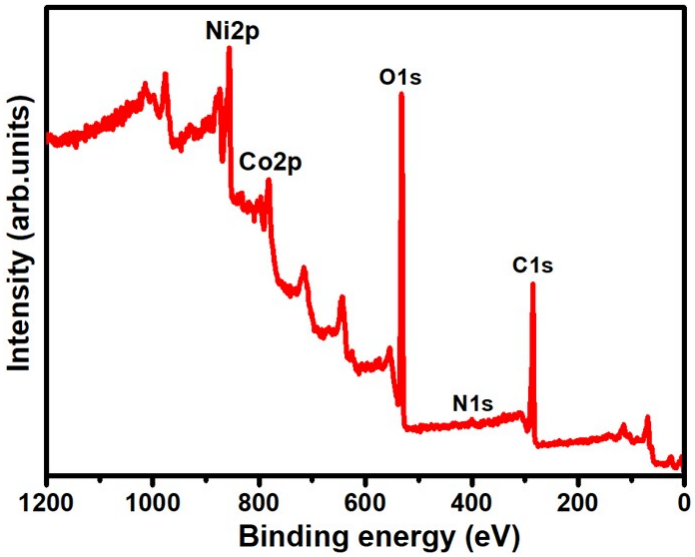

Figure S4. XPS survey spectrum of NiCoOOH@PANi-CF.

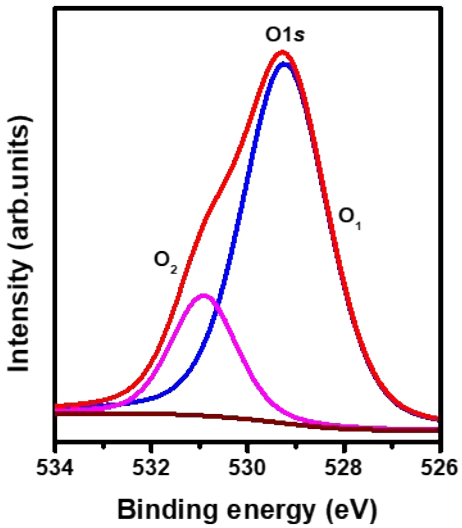

Figure S5. Deconvoluted O 1*s* XPS spectra of NiCoOOH@O-CF.

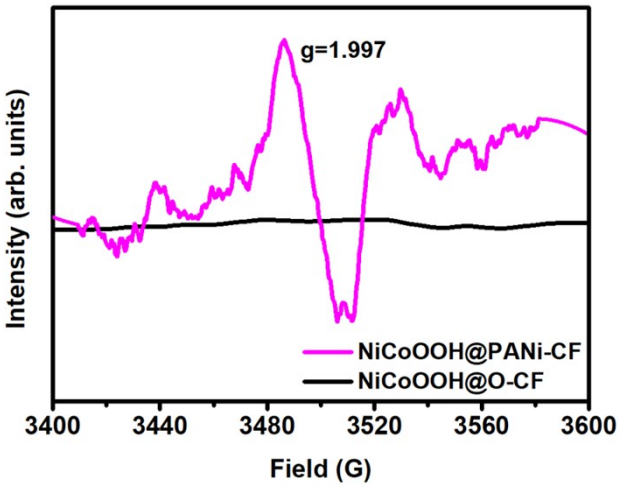

Figure S6. ESR measurement of NiCoOOH@PANi-CF and NiCoOOH@O-CF.

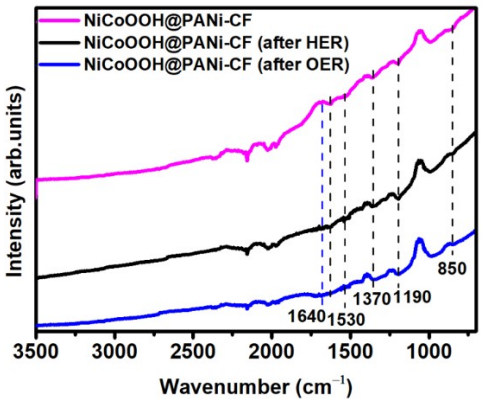

Figure S7. FTIR spectra of NiCoOOH@PANi-CF before and after HER/OER durability tests.

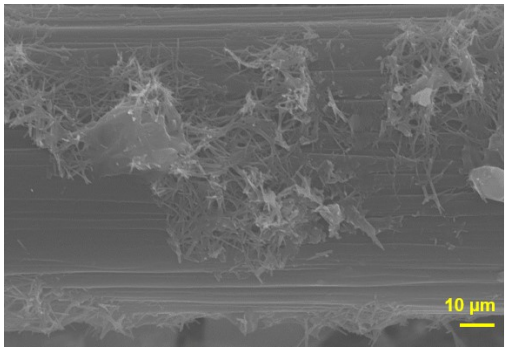

Figure S8. FESEM image of the NiCoOOH@O-CF after HER stability test in an acidic electrolyte.

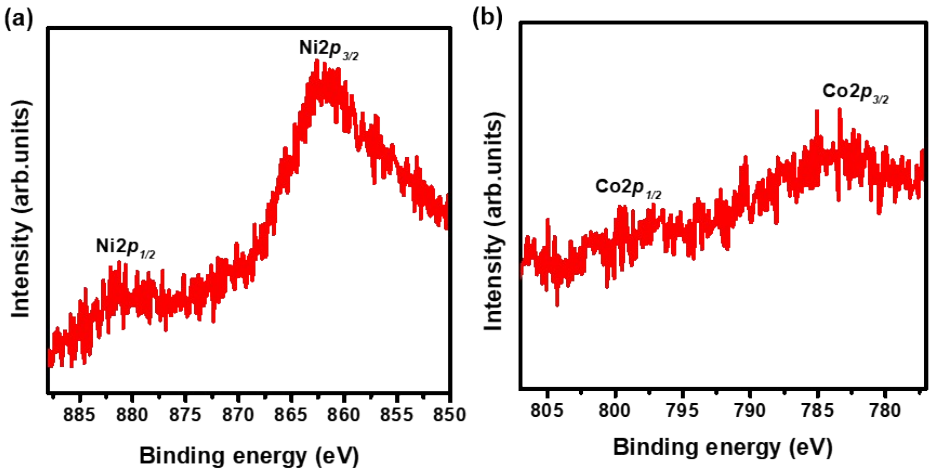

Figure S9. Deconvoluted (a) Ni 2*p* and (b) Co 2*p* XPS spectra of NiCoOOH@O-CF catalyst after HER stability test in an acidic electrolyte.

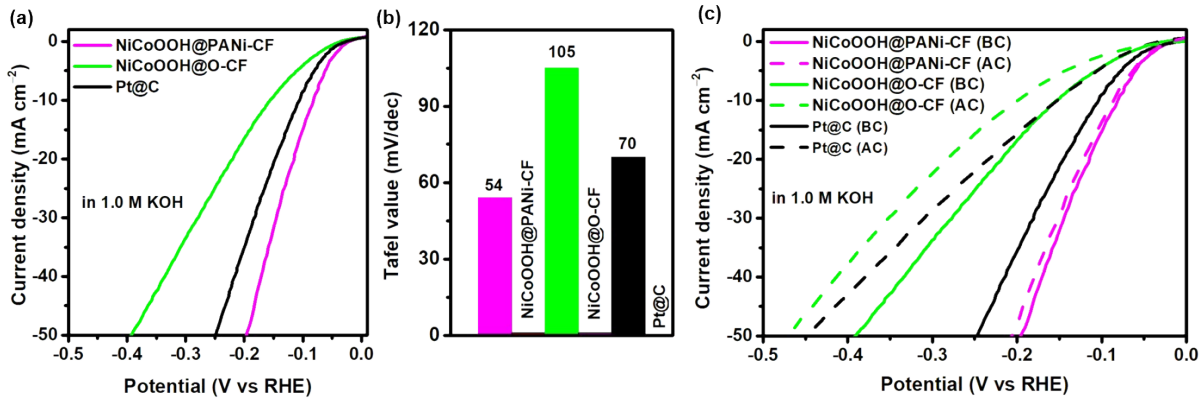

Figure S10. HER characteristics of NiCoOOH@PANi-CF in an alkaline electrolyte: (a) Polarization curves, (b) Tafel slope values, and (c) polarization curves before (BC) and after (AC) 2,000 cycles.

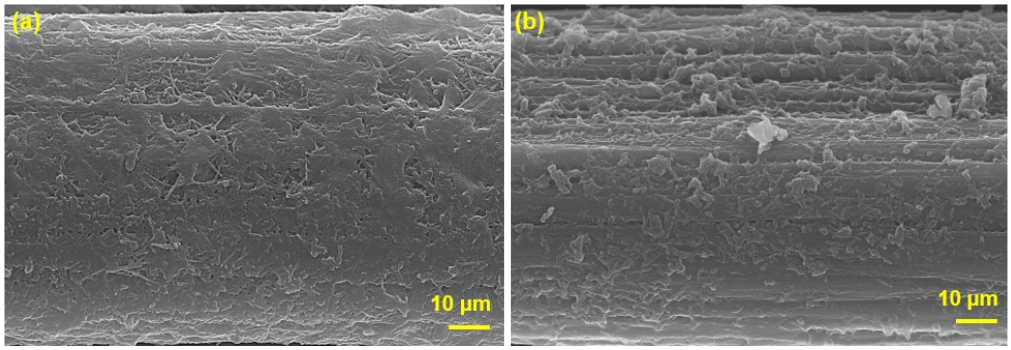

Figure S11. FESEM images of (a) NiCoOOH@PANi-CF and (b) NiCoOOH@O-CF after HER stability test in an alkaline electrolyte.

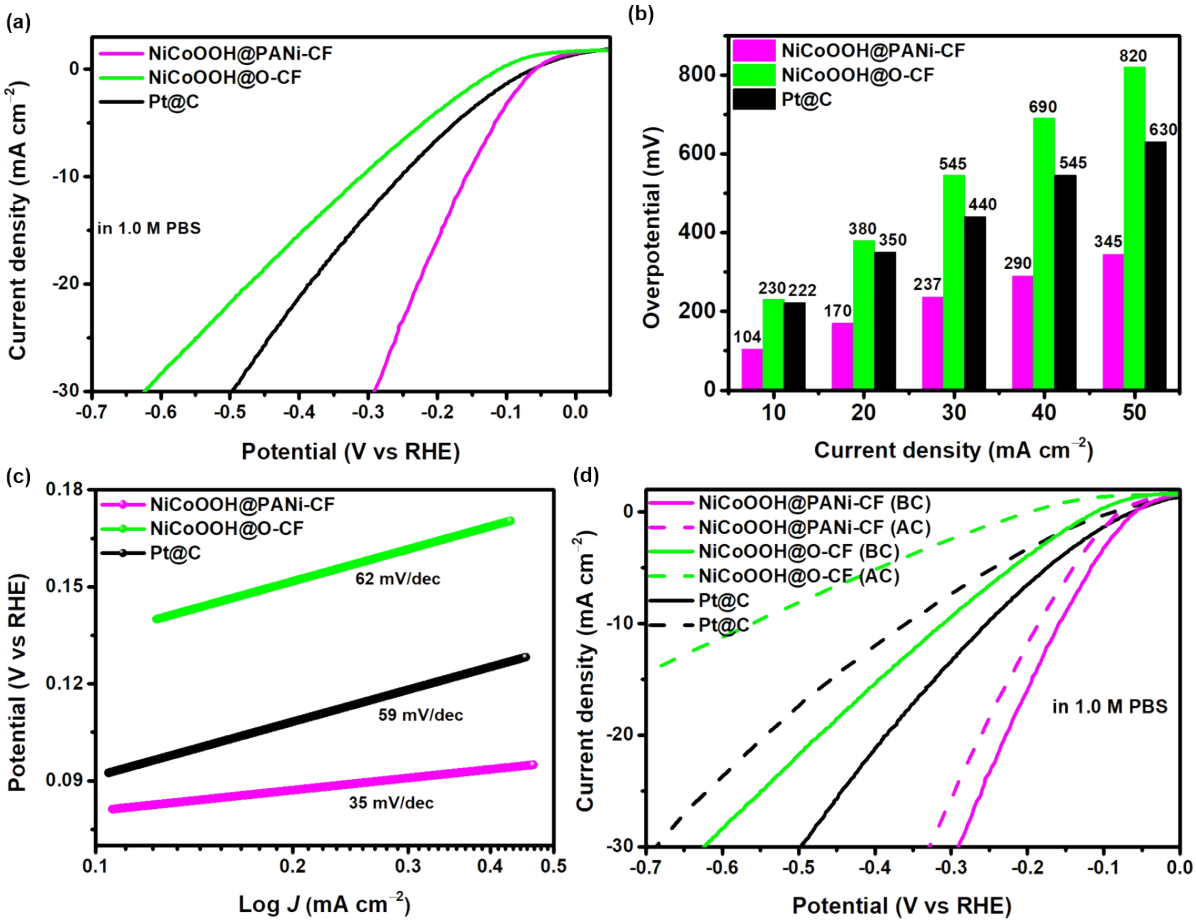

Figure S12. HER characteristics of NiCoOOH@PANi-CF in a neutral electrolyte: (a) Polarization curves, (b) overpotential value at different current densities, (c) Tafel plots, and (d) polarization curves before (BC) and after (AC) 2,000 cycles.

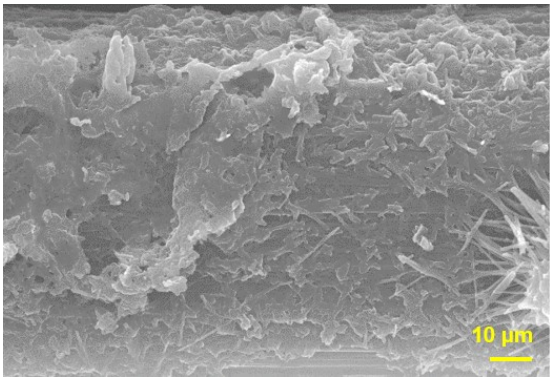

Figure S13. FESEM image of the NiCoOOH@O-CF after OER stability test in an alkaline electrolyte.

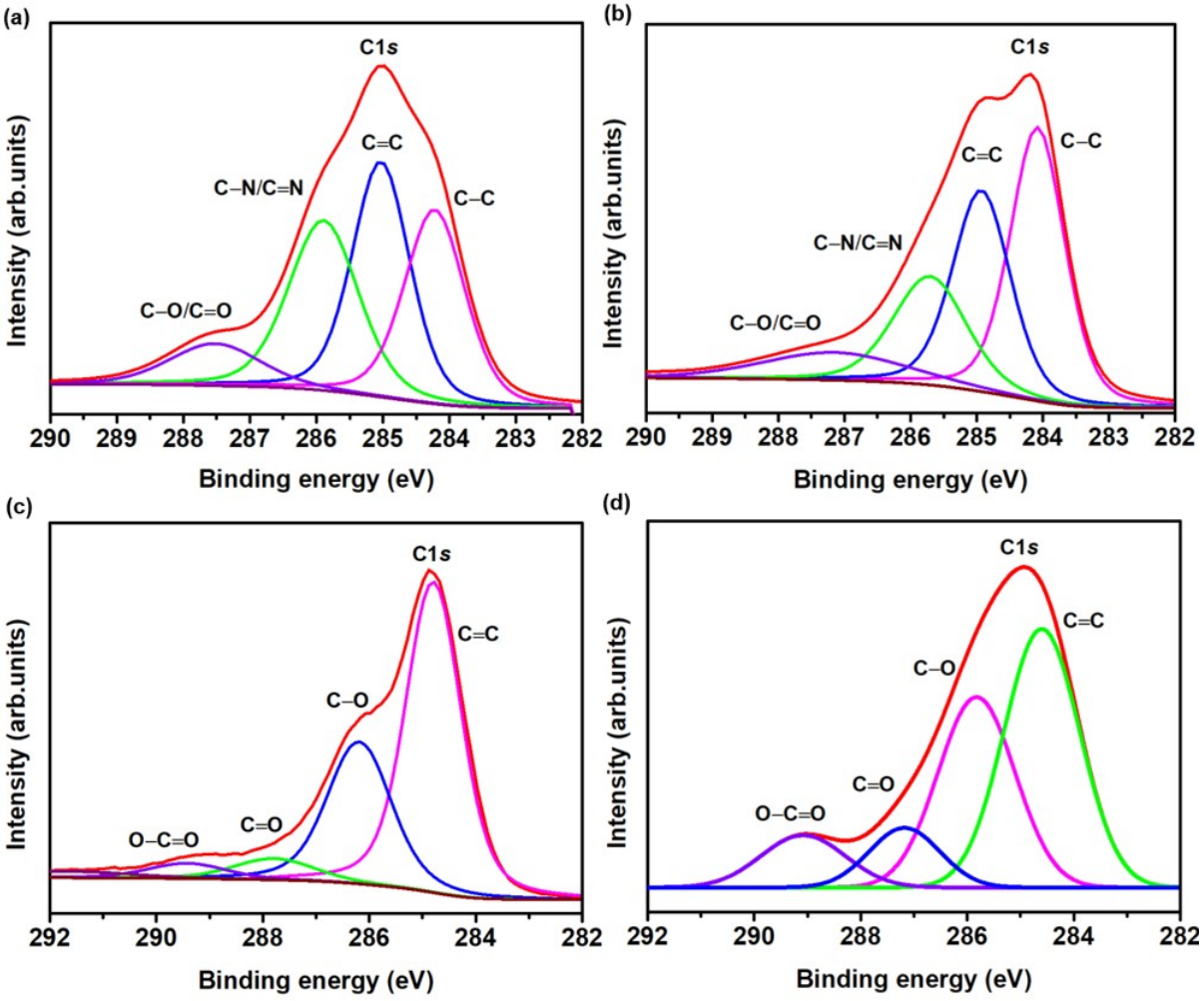

Figure S14. Deconvoluted C 1*s* XPS spectra of NiCoOOH@PANi-CF (a) before and (b) after OER stability tests in an alkaline electrolyte, and deconvoluted C 1*s* XPS spectra of the NiCoOOH@O-CF (c) before and (d) after OER stability tests in an alkaline electrolyte.

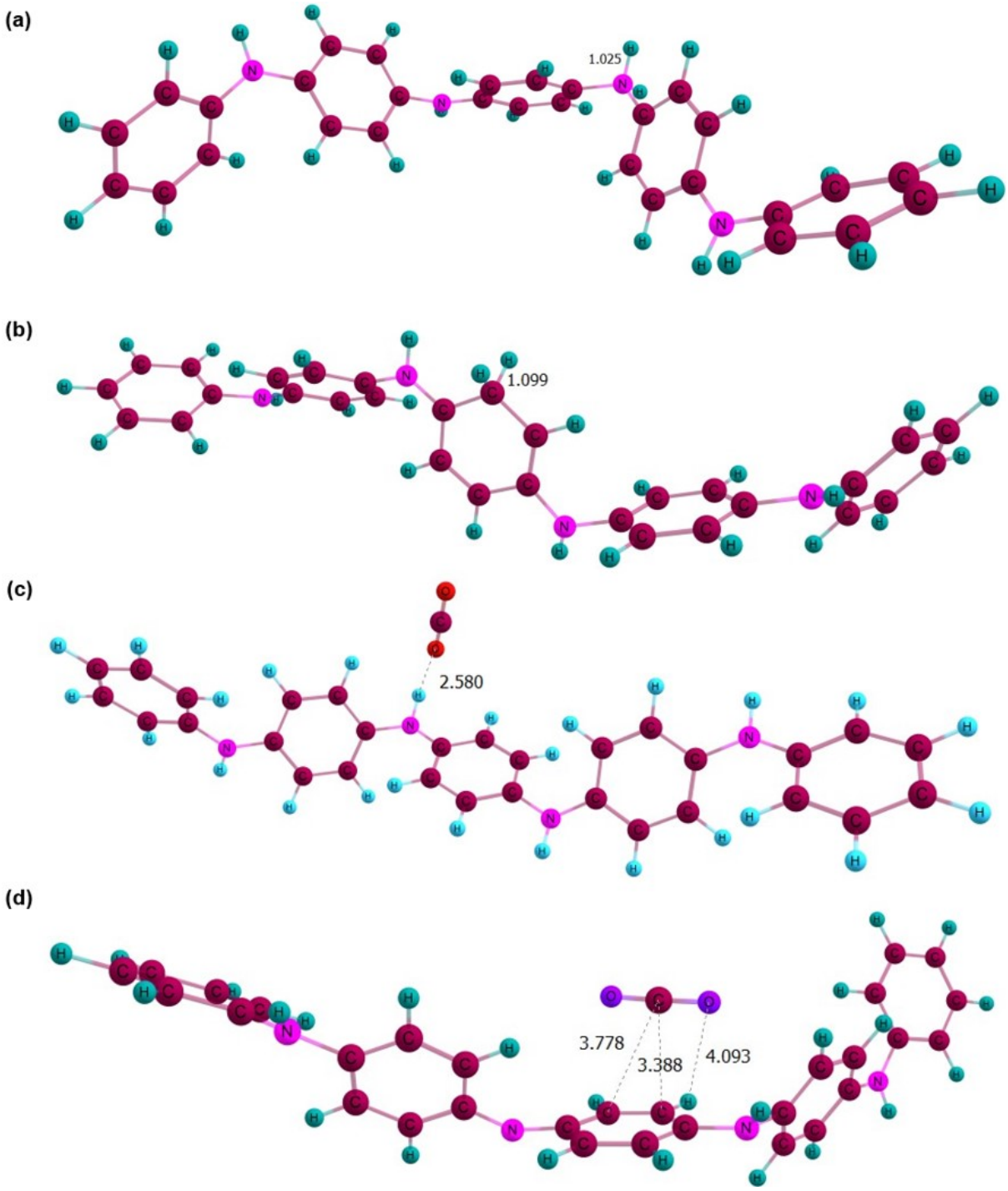

Figure S15. Adsorption of H^+ on (a) N atom and (b) C atom of PANi surface, and adsorption of CO_2 on (c) N atom and (d) C atom of PANi surface.

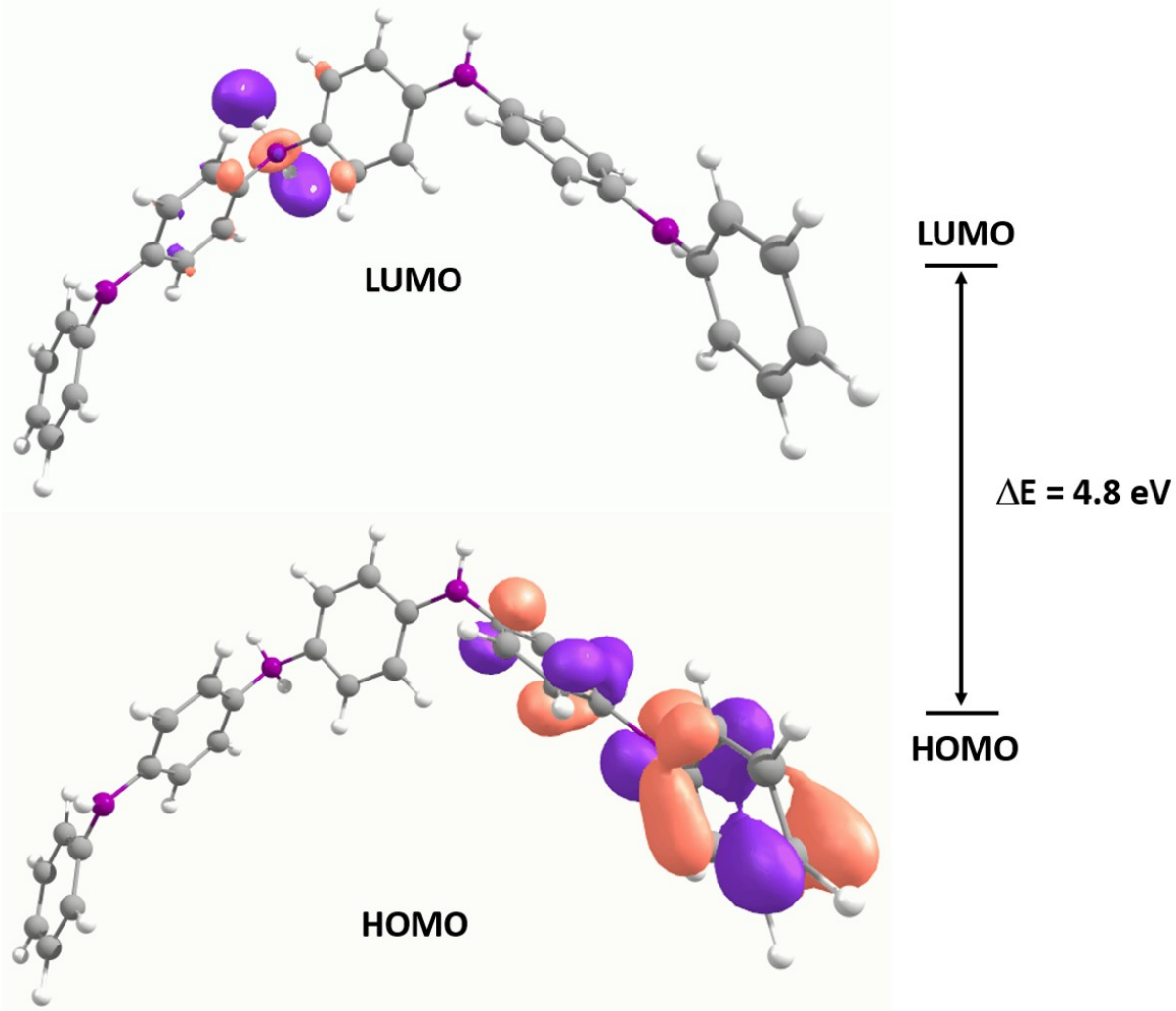

Figure S16. Molecular orbital (HOMO and LUMO) diagram and energy gap for H^+ ions adsorbed on PANi.

Samples	Overpotential [mV at 10 mA cm^{-2}]	Tafel slope [mV dec^{-1}]	Reference
Ferromagnetic MoS_2	64	59	[S1]
Ni-FeP/C	72	54	[S2]
1T-MoS_2	152	59	[S3]
CoP/NC	82	41	[S4]
CoP/MOF	27	43	[S5]
VN/Co-NC	22	31	[S6]
Ni-Se@NC	131	85	[S7]
VSe_2	67	45	[S8]
MoS_2 Nanomesh	160	46	[S9]
MoS_2/graphene	143	71	[S10]
MoS_2/vertical graphene/ carbon cloth	78	53	[S11]
NiCoOOH@PANi-CF	**35**	**37**	**This work**

Table S1. HER performance of various electrocatalysts in an acidic electrolyte.

Samples	Overpotential [mV at 10 mA cm^{-2}]	Tafel slope [mV dec^{-1}]	Reference
Ni-FeP/C	95	72	[S2]
CoP/NC	97	51	[S4]
CoP/MOF	34	56	[S5]
1T-2H MoS_2	290	42	[S12]
CoOX/CN	85	115	[S13]
$MoS_2/Co(OH)_2$	89	53	[S14]
La-Co_3O_4	98	72	[S15]
Co_3O_4/NC	310	60	[S16]
N-doped Co_2P/CC	34	51	[S17]
Sulfurized NiMnLDH	93	80	[S18]
$MoS_2@Ni_2P$	95	42	[S19]
Mo_2C@NPCS	147	77	[S20]
Co@NiS_2	80	43	[S21]
Co-Fe-P	86	66	[S22]
CeO_2/Co_4N	30	66	[S23]
CoP/MoO_2	42	73	[S24]
MoP/N,P-G	126	56	[S25]
S-$NiFeSO_4$	61	80	[S26]
CoP/CoMoP	34	33	[S27]
Co_3S_4/MoS_2	90	62	[S28]
CoP_3/CoMoP/NF	110	64	[S29]
Carbon doped CoP	30	37	[S30]
NiV-LDH/NF	114	87	[S31]
Cobalt/N-graphene	172	48	[S32]
PSS/PPY@Ni-Co-P	67	27	[S33]
Nanoporous CoP/S	103	58	[S34]
C/NiO	27	36	[S35]
MoC/NC	160	39	[S36]
NiCoOOH@PANi-CF	**30**	**54**	**This work**

Table S2. HER performance of various electrocatalysts in an alkaline electrolyte.

Samples	Overpotential [mV at 10 mA cm^{-2}]	Tafel slope [mV dec^{-1}]	Reference
Ni-FeP/C	117	70	[S2]
CoP/Co-MOF	49	43	[S5]
VN/Co-NC	163	117	[S6]
Ni-Se@NC	183	135	[S7]
VSe_2	122	66	[S8]
N-doped Co_2P/CC	42	68	[S17]
Co-Fe-P	138	138	[S22]
MoP/N,P-G	150	102	[S25]
CoP_3/CoMoP/NF	89	97	[S29]
NiV-LDH/NF	114	44	[S31]
PSS/PPY@Ni-Co-P	106	81	[S33]
CoNi/Co-NiLDH	145	80	[S37]
W@MoP	82	74	[S38]
Co_9S_8/MoS_2	152	99	[S39]
FeS	78	136	[S40]
W-CoP	102	87	[S41]
CoWS	198	94	[S42]
NiCoP	97	87	[S43]
Ni_2P/N-CNF	185	230	[S44]
Mo_5N_6/MoS_2	59	43	[S45]
Ni_3N/VN	85	73	[S46]
Ni_3S_2/NC	249	78	[S47]
P-doped Co_2MnO_4	102	143	[S48]
CoP/NiCoP/NC	123	78	[S49]
N,S,O-C/Co_9S_8	103	113	[S50]
NiCoOOH@PANi-CF	**110**	**35**	**This work**

Table S3. HER performance of various electrocatalysts in a neutral electrolyte.

Samples	Overpotential [mV at 10 mA cm^{-2}]	Tafel slope [mV dec^{-1}]	Reference
Oxygen rich NiFeLDH	310	74	[S51]
CoMoOS	281	75.4	[S52]
Vacancy rich NiFeLDH	195	47.9	[S53]
Edge rich NiFeLDH	205	41.8	[S54]
LiNiFe borophosphate	215	37	[S55]
Single atom Ni	224	42	[S56]
NiFeCr/NF	240	36	[S57]
CoP/CeO_2	224	90.3	[S58]
$NiSe_2/FeSe_2$	256	50	[S59]
Ni_5P_4/FeP	205	42.3	[S60]
NiCoOOH@PANi-CF	**20**	**41**	**This work**

Table S4. OER performance of various electrocatalysts in an alkaline electrolyte.

Samples	Overpotential [V vs RHE at 10 mA cm^{-2}]	Tafel slope [mV dec^{-1}]	Reference
CoFe nanoneedles	1.3	40	[S61]
NF/NiMoO-Ar	1.5	19	[S62]
F-NiO/Ni@C	1.31	37	[S63]
P-$NiMoO_4$	1.35	19	[S64]
P-$CoNi_2S_4$	1.306	55	[S65]
Ni_2P/Fe_2P	1.36	79	[S66]
NiCoP/CC	1.30	49	[S67]
NiP/NiO-NiPi	1.44	70	[S68]
Nickel terephthalate	1.38	52	[S69]
$Ni@Co_9S_8$	1.28	56	[S70]
$Co_3O_4@Co_2P_4O_{12}$	1.31	126	[S71]
CoNi oxyphosphides	1.29	106	[S72]
$Fe_2P@Ni_xP/NF$	1.34	30	[S73]
$Ni_3N/Ni_{0.2}Mo_{0.8}N$	1.32	17	[S74]
NiCoOOH@PANi-CF	**1.32**	**53**	**This work**

Table S5. UOR performance of various electrocatalysts in 1.0 M KOH/0.33 M urea electrolyte.

Table S6. Calculated energies of H^+ ions and CO_2 on PANi surface by M06-2X/6-311++G(d,p) level of theory.

Species	E [eV]	H_{298} [eV]	G_{298} [eV]
PANi	−1377.638898	−1377.117323	−1377.213859
CO_2	−188.574880	−188.559341	−188.583564
PANi–H–C (PANi–H^+)	−1377.995982	−1377.461703	−1377.557762
PANi–H–N (PANi–H^+)	−1378.013922	−1377.477582	−1377.573554
PANi–CO_2–C (PANi–CO_2) Conformer 1	−1566.222791	−1565.684202	−1565.790257
PANi–CO_2–C (PANi–CO_2) Conformer 2	−1566.222791	−1565.684200	−1565.790259
PANi–CO_2–N (PANi–CO_2)	−1566.222791	−1565.684197	−1565.790228

Table S7. Calculated adsorption energies for H^+ ions and CO_2 adsorption on PANi surface by M06-2X/6-311++G(d,p) level of theory.

Species	ΔE [eV]	ΔH_{298} [eV]	ΔG_{298} [eV]
PANi–H–C (PANi–H^+)	−9.75	−9.37	−9.35
PANi–H–N (PANi–H^+)	−10.2	−9.80	−9.78
PANi–CO_2–C (PANi–CO_2)	−0.24	−0.20	0.19
PANi–CO_2–N (PANi–CO_2)	−0.24	−0.20	0.19

Table S8. Mulliken charges for H^+ ions and CO_2 on PANi.

Atoms	Before adsorption		After adsorption	
	PANi	H^+	PANi in PANi–H^+	H^+ in PANi–H^+
C	0.094869	1.000000	0.009358	−0.092468
N	0.125035	1.000000	0.183854	−0.064150
	PANi	CO_2	PANi in PANi– CO_2	CO_2 in PANi– CO_2
C	0.118980	0.521310	0.168452	0.312106
N	0.125035	0.521310	0.175849	−0.044828

Samples	Urea electrolysis [V vs. RHE at 10 mA cm^{-2}]	Water electrolysis [V vs. RHE at 10 mA cm^{-2}]	Reference
CoFe-250	1.30	1.47	[S70]
N-Co_9S_8/Ni_3S_2/NF	1.40	1.55	[S75]
Mo-Ni/NiO	1.45	1.65	[S76]
Mo-FeNi LDH	1.39	1.49	[S77]
NiFeMo	1.46	1.60	[S78]
NC-PB@CNT	1.34	1.61	[S79]
Ni/MoC/$Ti_3C_2T_x$@C	1.56	1.64	[S80]
Ru-$NiCo_2O_4$	1.42	1.55	[S81]
CoO–Co_4N@NiFe-LDH/NF	1.39	1.52	[S82]
$Fe_{11.1\%}$–Ni_3S_2/Ni foam	1.46	1.60	[S83]
$FeNi_2S_4$/CoFe	1.56	1.72	[S84]
V/meso-Co/NF-5	1.39	1.63	[S85]
Ce-Ni_2P	1.51	1.62	[S86]
$NiCo_2S_4$ NS/CC	1.49	1.7	[S87]
NiCoOOH@PANi-CF	**1.39**	**1.51**	**This work**

Table S9. Full cell performance of various electrocatalysts for water and urea splitting.

References for Supporting Information

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