Supporting Information for

Nb-doped Nickel Nitride-Derived Catalysts for Electrochemical Water Splitting

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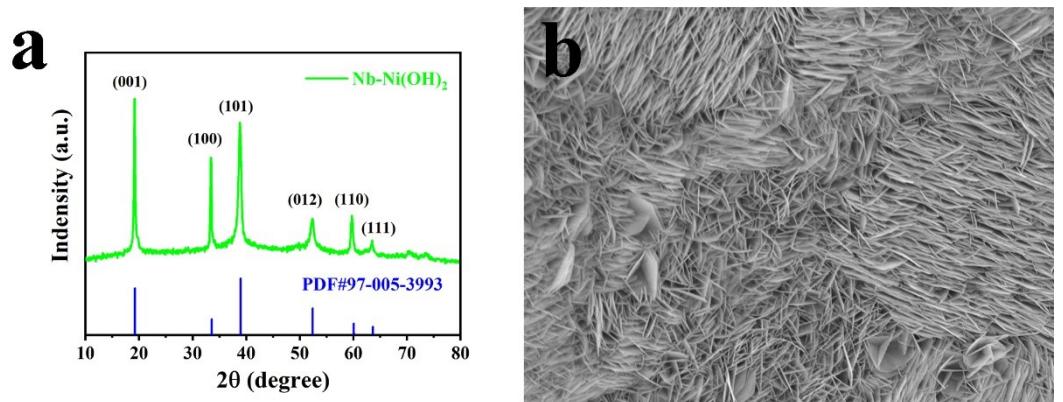
Fig. S1. (a) XRD pattern of Nb-Ni(OH)$_2$. (b) SEM image of Nb-Ni(OH)$_2$/NF.
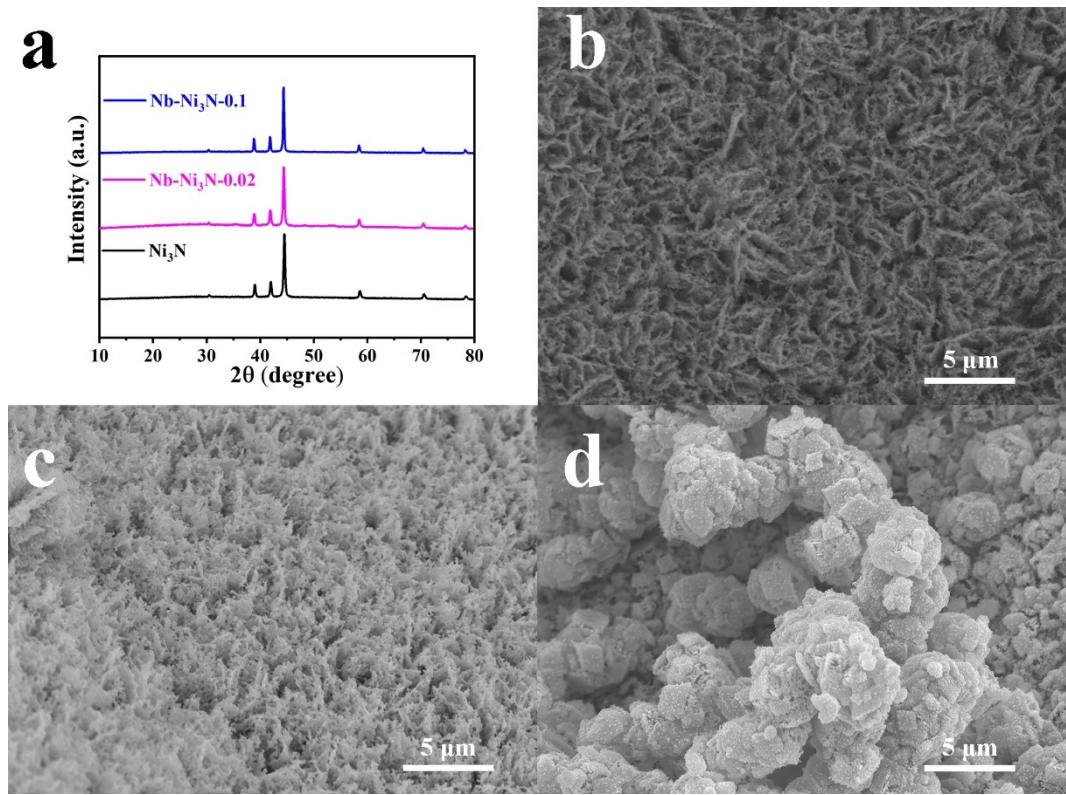
**Fig. S2.** a) XRD patterns, b) SEM image of undoped Ni_3N. c) SEM image of Nb-Ni_3N-0.02, d) SEM image of Nb-Ni_3N-0.1.
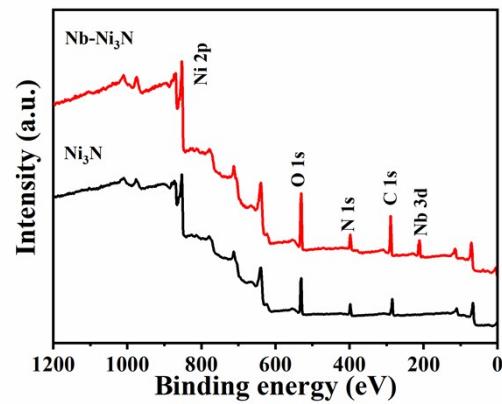


Fig. S3 The XPS survey spectra.
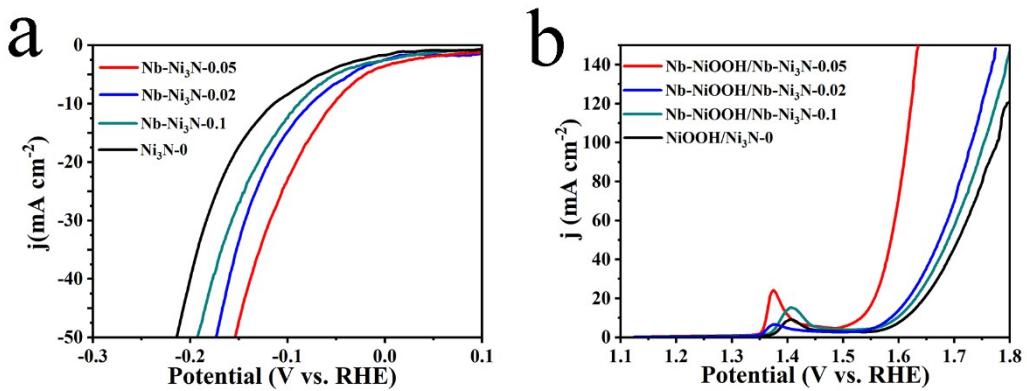
Fig. S4. (a) LSV curve of Nb-Ni$_3$N-x/NF (x= 0, 0.02, 0.05,0.1) for HER. (b) LSV curve of Nb-NiOOH/Nb-Ni$_3$N-x (x= 0, 0.02, 0.05,0.1) for OER.
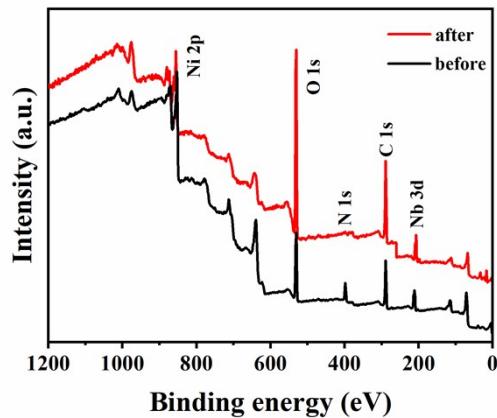
Fig S5. XPS full survey spectra of Nb-Ni$_3$N/NF before and after 3-h OER stability test.

Table S1. EIS fitting parameters from equivalent circuit of samples for HER at 50 mV overpotential and OER at 300 mV overpotential.

samples	R_{ct}	R_s	CPE-T	CPE-P
Nb-Ni$_3$N-0.05	6.41	1.054	0.019971	0.75294
Ni$_3$N	14.16	1.197	0.02055	0.77825
Nb-NiOOH/Ni$_3$N-0.05	6.38	1.054	0.18806	0.53487
NiOOH/Ni$_3$N	10.14	1.102	0.095753	0.69642
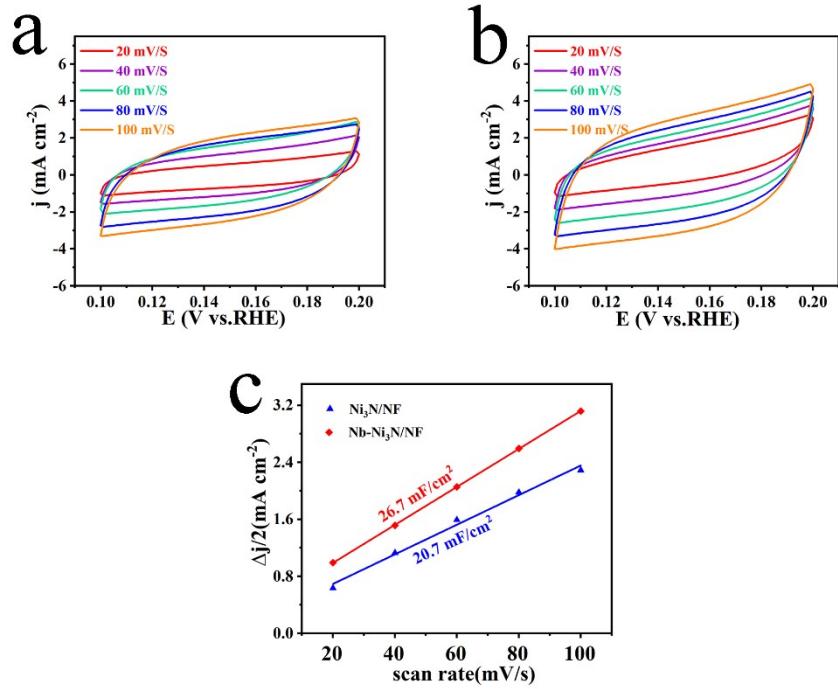
Fig S6. CV scans for HER of (a) Ni_3N/NF, (b) $Nb-Ni_3N-0.05/NF$ and (c) the capacitive current at 0.15 V vs. RHE.
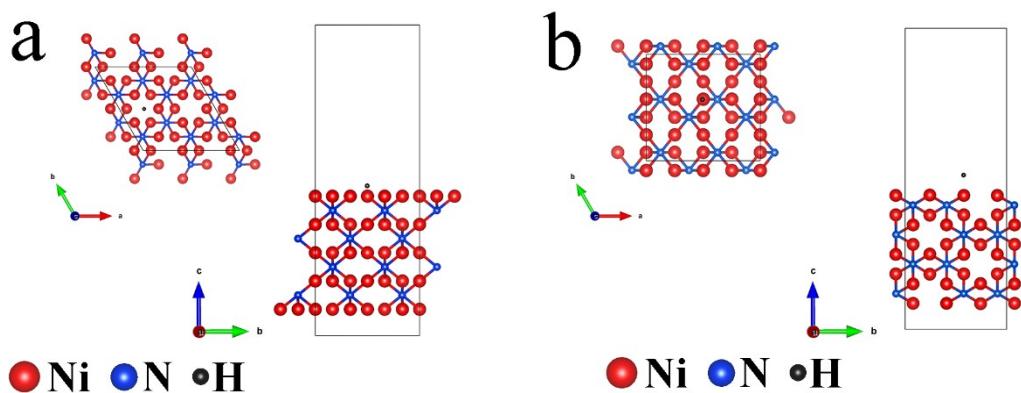
Fig. S7 (a) the geometric configuration of Ni_3N (002). (b) the geometric configuration of Ni_3N (110).

Table S2. atomic coordinates of Nb-Ni$_3$N (002)

	X	Y	Z
Ni1	0.08357	0.33595	0.08751
Ni2	0.06843	0.32738	0.2621
Ni3	0.07466	0.3415	0.45013
Ni4	0.40919	0.16845	0.17502
Ni5	0.40926	0.15367	0.36025
Ni6	0.07832	-0.00319	0.17463
Ni7	0.07599	-0.00747	0.35889
Ni8	0.23723	0.15719	0.08746
Ni9	0.23381	0.15129	0.264
Ni10	0.25319	0.16132	0.44981
Ni11	0.40718	0.00688	0.08758
Ni12	0.40836	0.00899	0.26386
Ni13	0.40091	-0.01045	0.4465
Ni14	0.24108	0.33221	0.17377
Ni15	0.58564	0.3354	0.08728
Ni16	0.58664	0.33581	0.26151
Ni17	0.57804	0.33686	0.44811
Ni18	0.90797	0.1665	0.17427
Ni19	0.90329	0.15916	0.35924
Ni20	0.57806	-0.00245	0.17434
Ni21	0.58577	0.01024	0.35726
Ni22	0.73847	0.15882	0.08787
Ni23	0.73493	0.15633	0.26402
Ni24	0.75155	0.16477	0.44703
Ni25	0.90753	0.00517	0.0878
Ni26	0.91098	0.00224	0.26659
Ni27	0.88774	-0.01907	0.44907
Ni28	0.74539	0.33401	0.17439
Ni29	0.73822	0.3212	0.35999
Ni30	0.0853	0.83621	0.08768
Ni31	0.07707	0.83082	0.26654
Ni32	0.07684	0.85206	0.44819
Ni33	0.41205	0.6699	0.17028
Ni34	0.07879	0.50042	0.17549
Ni35	0.23743	0.65955	0.0872
Ni36	0.24066	0.66892	0.26593
Ni37	0.25169	0.66726	0.45184
Ni38	0.40701	0.50367	0.08775
Ni39	0.40432	0.48712	0.44976
Ni40	0.243	0.83571	0.1751
Ni41	0.24069	0.84277	0.35894

Ni42	0.5849	0.83751	0.08738
Ni43	0.58362	0.84087	0.26523
Ni44	0.58143	0.85492	0.45023
Ni45	0.90794	0.66642	0.17409
Ni46	0.91494	0.67553	0.35662
Ni47	0.58218	0.49911	0.17262
Ni48	0.73906	0.65915	0.0873
Ni49	0.74576	0.66742	0.26654
Ni50	0.76835	0.67044	0.45194
Ni51	0.90777	0.50433	0.08812
Ni52	0.90542	0.50278	0.26438
Ni53	0.89555	0.49201	0.44774
Ni54	0.75235	0.84376	0.17308
Ni55	0.75235	0.84487	0.35757
Nb1	0.23588	0.31277	0.3618
Nb2	0.42076	0.68903	0.3631
Nb3	0.06597	0.49949	0.35934
Nb4	0.40532	0.50078	0.26215
Nb5	0.59789	0.5001	0.36254
N1	0.4102	0.33212	0.12344
N2	0.4182	0.31664	0.30854
N3	0.07313	0.16106	0.21777
N4	0.06204	0.14945	0.41695
N5	0.9105	0.33388	0.12474
N6	0.89752	0.31871	0.30851
N7	0.578	0.16456	0.21663
N8	0.57537	0.16131	0.41071
N9	0.40927	0.83627	0.12368
N10	0.40884	0.84835	0.30902
N11	0.07399	0.66763	0.21815
N12	0.0781	0.67913	0.41518
N13	0.91151	0.83363	0.12396
N14	0.91262	0.83834	0.31086
N15	0.58612	0.67662	0.21595
N16	0.59606	0.67652	0.4173
H1	0.247	0.499	0.48305

Table S3. atomic coordinates of Nb-Ni$_3$N (110)

	X	Y	Z
Ni1	0.00026	0.74334	0.1495
Ni2	0.00013	0.24387	0.25057
Ni3	0.0072	0.73989	0.34825
Ni4	-0.00335	0.24637	0.44437
Ni5	0.24979	0.74341	0.08986
Ni6	0.25029	0.24336	0.18238
Ni7	0.24859	0.73929	0.27913
Ni8	0.25163	0.08059	0.09066
Ni9	0.24973	0.57984	0.18379
Ni10	0.25034	0.08049	0.28167
Ni11	0.24765	0.58037	0.38131
Ni12	-0.00003	0.07601	0.14883
Ni13	-0.00127	0.57943	0.24824
Ni14	-0.00541	0.08185	0.34499
Ni15	0.00125	0.58894	0.4407
Ni16	-0.0002	0.41142	0.14896
Ni17	0.00364	0.90812	0.24728
Ni18	0.00522	0.40908	0.34594
Ni19	-0.00745	0.90169	0.44315
Ni20	0.24752	0.40732	0.0908
Ni21	0.25045	0.90757	0.18383
Ni22	0.24772	0.40954	0.28062
Ni23	0.50027	0.74334	0.1495
Ni24	0.50022	0.24416	0.25072
Ni25	0.5073	0.73917	0.34827
Ni26	0.49776	0.24777	0.44507
Ni27	0.74977	0.74346	0.08988
Ni28	0.75025	0.24327	0.18236
Ni29	0.74872	0.7395	0.27904
Ni30	0.75166	0.08056	0.09063
Ni31	0.74972	0.57981	0.18379
Ni32	0.75041	0.08054	0.2817
Ni33	0.74756	0.58098	0.38113
Ni34	0.50003	0.07602	0.14882
Ni35	0.49872	0.57923	0.24818
Ni36	0.49485	0.08189	0.34522
Ni37	0.4993	0.58752	0.44584
Ni38	0.4998	0.4114	0.14894
Ni39	0.5037	0.90814	0.24721
Ni40	0.50384	0.41192	0.34722
Ni41	0.49309	0.89803	0.44488

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Ni42	0.74757	0.40729	0.09078
Ni43	0.75044	0.90762	0.18381
Ni44	0.74777	0.40969	0.28065
Nb1	0.24609	0.25057	0.37786
Nb2	0.25604	0.88823	0.38722
Nb3	0.74656	0.25102	0.37806
Nb4	0.75446	0.88806	0.38714
N1	0.12758	0.57473	0.11541
N2	0.12393	0.07732	0.21492
N3	0.12774	0.57676	0.31331
N4	0.12204	0.07554	0.42257
N5	0.37179	0.91241	0.11562
N6	0.37635	0.41093	0.21537
N7	0.37696	0.90527	0.31162
N8	0.38038	0.42114	0.4191
N9	0.62761	0.57473	0.11543
N10	0.62392	0.07729	0.21494
N11	0.62811	0.5769	0.31342
N12	0.61994	0.07459	0.42271
N13	0.87185	0.91237	0.11561
N14	0.87636	0.41089	0.21534
N15	0.87682	0.9053	0.31161
N16	0.87845	0.42059	0.41992
H1	0.49431	0.57899	0.50967
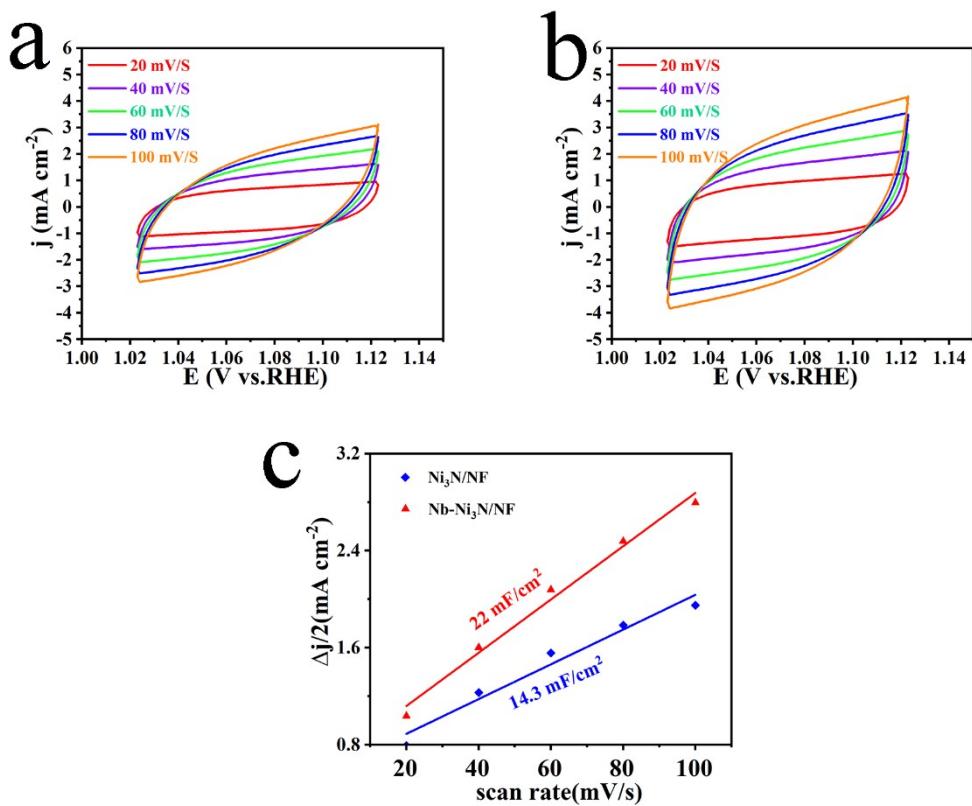
Fig S8. CV scans for OER of (a) Ni_3N/NF, (b) $Nb-Ni_3N-0.05/NF$ and (c) the capacitive current at 1.073 V vs. RHE.

Table S4. Comparison of the HER and/or OER performance of Nb-Ni$_3$N/NF with other reported electrocatalysts.

Catalysts	Electrolytes	HER		OER		Reference
		η_{10} (mV)	Tafel slope (mV dec^{-1})	η_{10} (mV)	Tafel slope (mV dec^{-1})	
Ni$_3$N/NF	1M KOH	121	109	-	-	1
Ni$_3$N/C	1M KOH	64	48	-	-	2
TiN@Ni$_3$N	1M KOH			350	93.7	3
Ni$_3$N-VN/NF	1M KOH	64	37			4
NiCoN NWs	1M NaOH	145	105.2	360	46.9	5
Epitaxial in-growth Co-Ni$_3$N	1M KOH	-	-	304	57	6
Nb-Ni$_3$N/NF	1M KOH	53	112	302	75	This work

References

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