Supporting information

Porous single crystal microcubes of niobium nitride for highly efficient electrocatalysis

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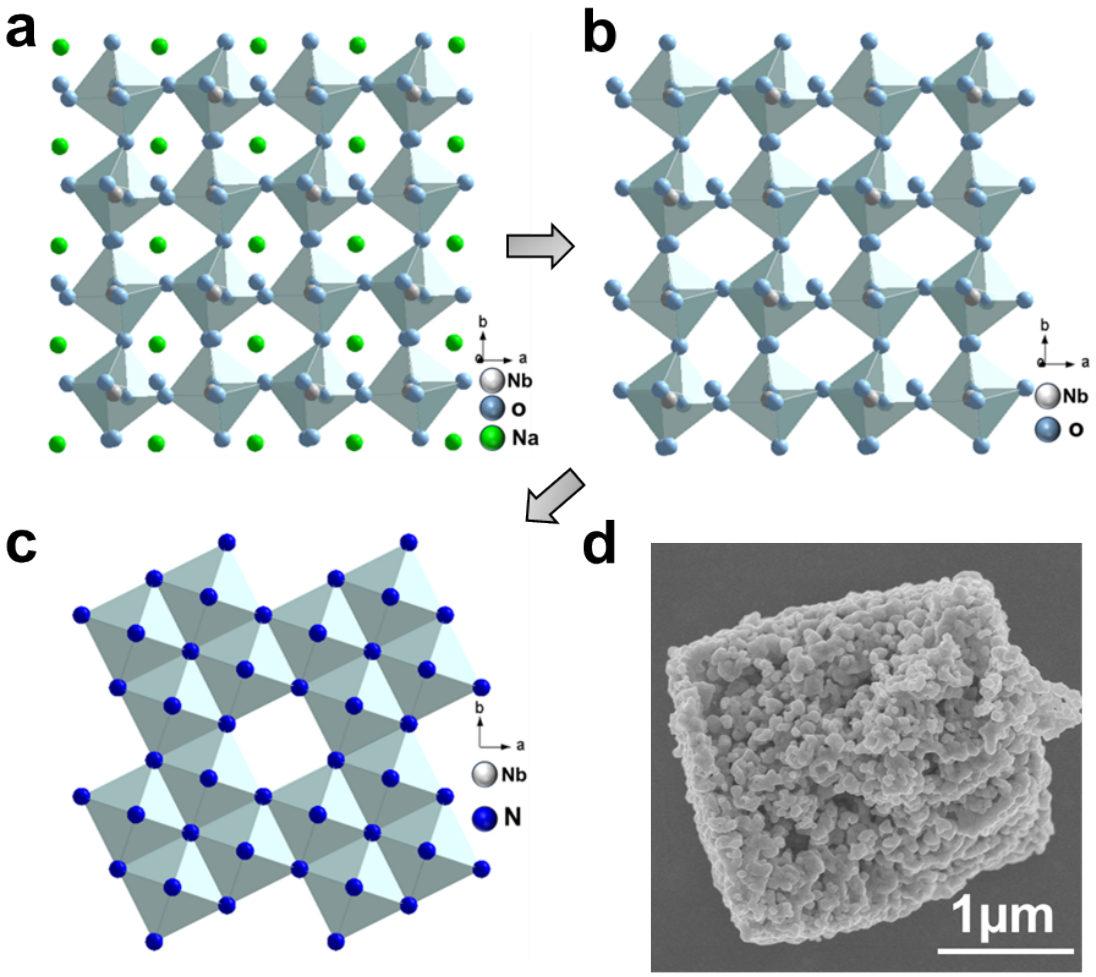
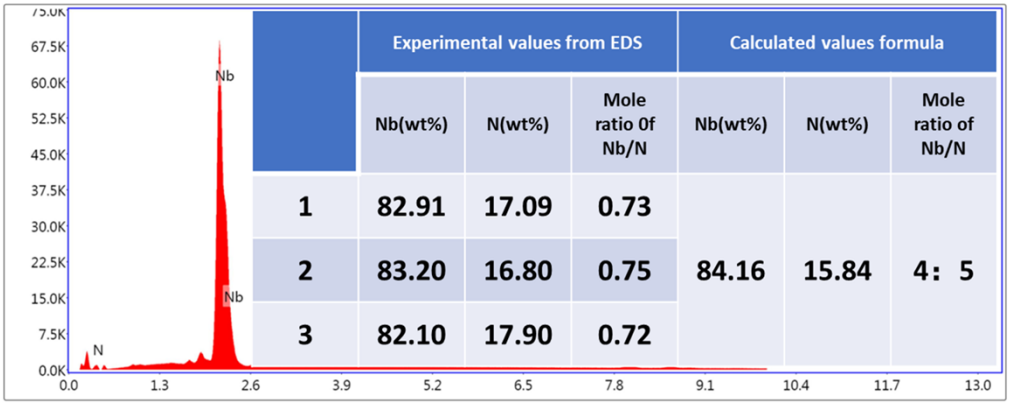


Fig. S1 (a) The lattice channel of atomic evaporation of the (100) facet of $NaNbO_3$ substrates. (b) (100) orientation of $NaNbO_3$ single crystal after evaporation of Na atoms. (c) (001) orientation of PSC Nb_4N_5 monoliths (Na atoms are green, O atoms are gray, Nb atoms are white, N atoms are blue). (d) SEM image of PPC Nb_4N_5



	Experimental values from EDS			Calculated values formula		
	Nb(wt%)	N(wt%)	Mole ratio 0f Nb/N	Nb(wt%)	N(wt%)	Mole ratio of Nb/N
1	82.91	17.09	0.73	84.16	15.84	4: 5
2	83.20	16.80	0.75			
3	82.10	17.90	0.72			

Fig. S2 The element analysis of PSC Nb_4N_5. No oxygen residual is observed from EDS elemental analysis. The mole ratio between Nb and N is approximately at 4:5.

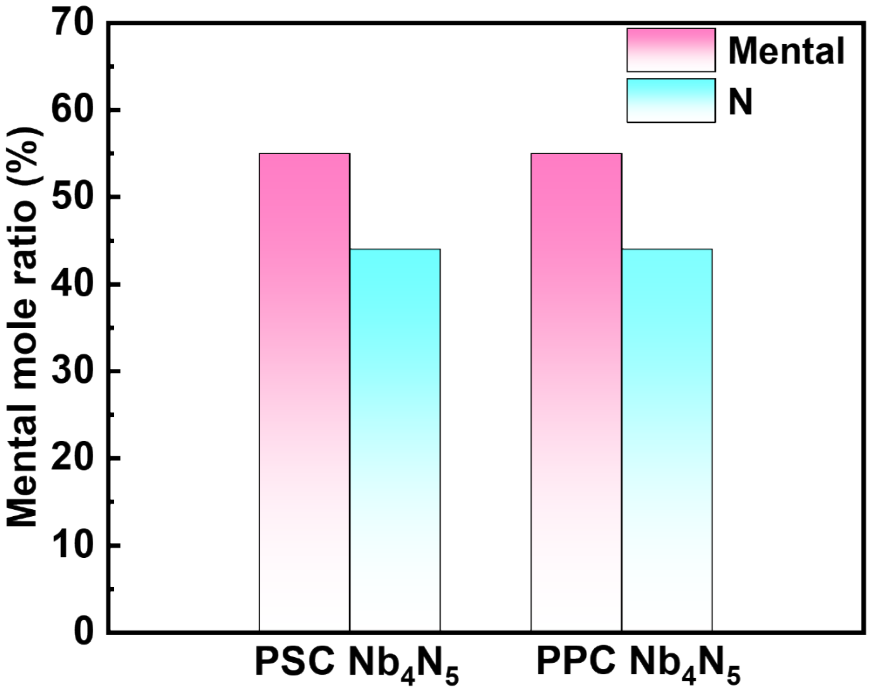


Fig. S3 ICP and CA results. Mole ratio between metal and nitrogen in PSC Nb_4N_5 and PPC Nb_4N_5.

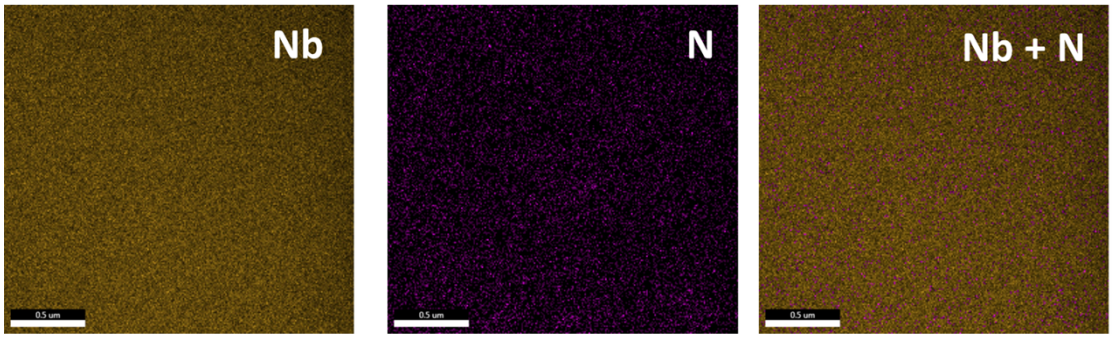


Fig. S4 EDS mapping images of PSC Nb_4N_5.

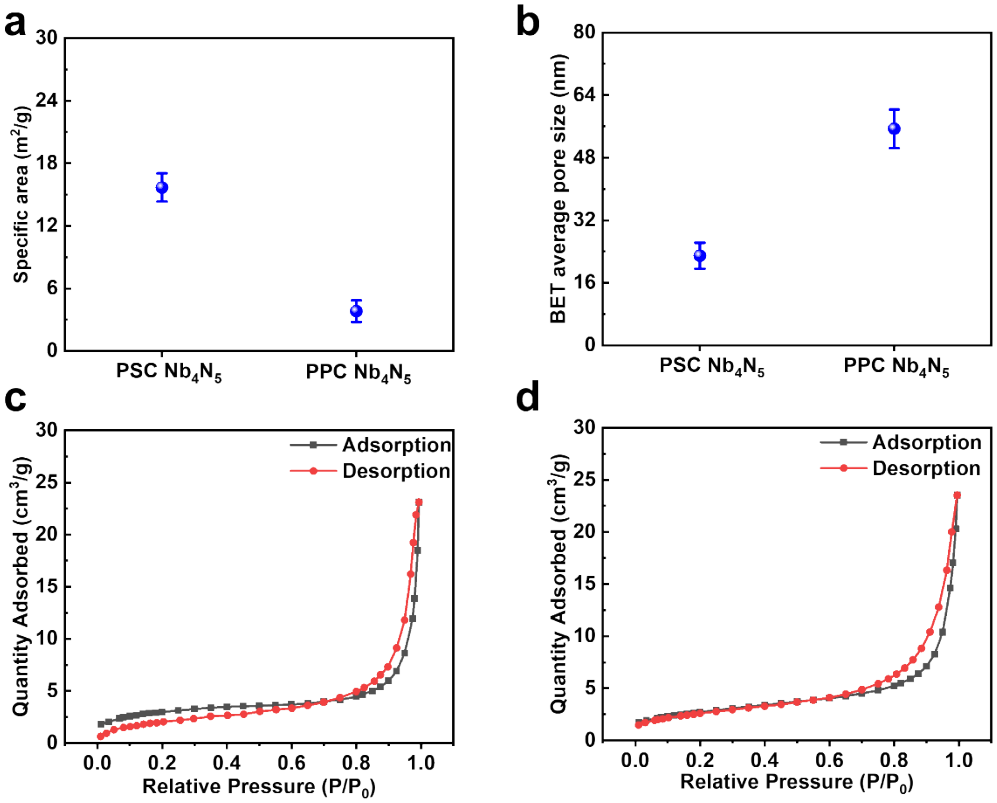


Fig. S5 (a, b) The surface specific area and BET average pore size of PSC Nb_4N_5 and PPC Nb_4N_5. (c) Nitrogen adsorption-desorption isotherm of PSC Nb_4N_5. (d) Nitrogen adsorption-desorption isotherm of PPC Nb_4N_5.

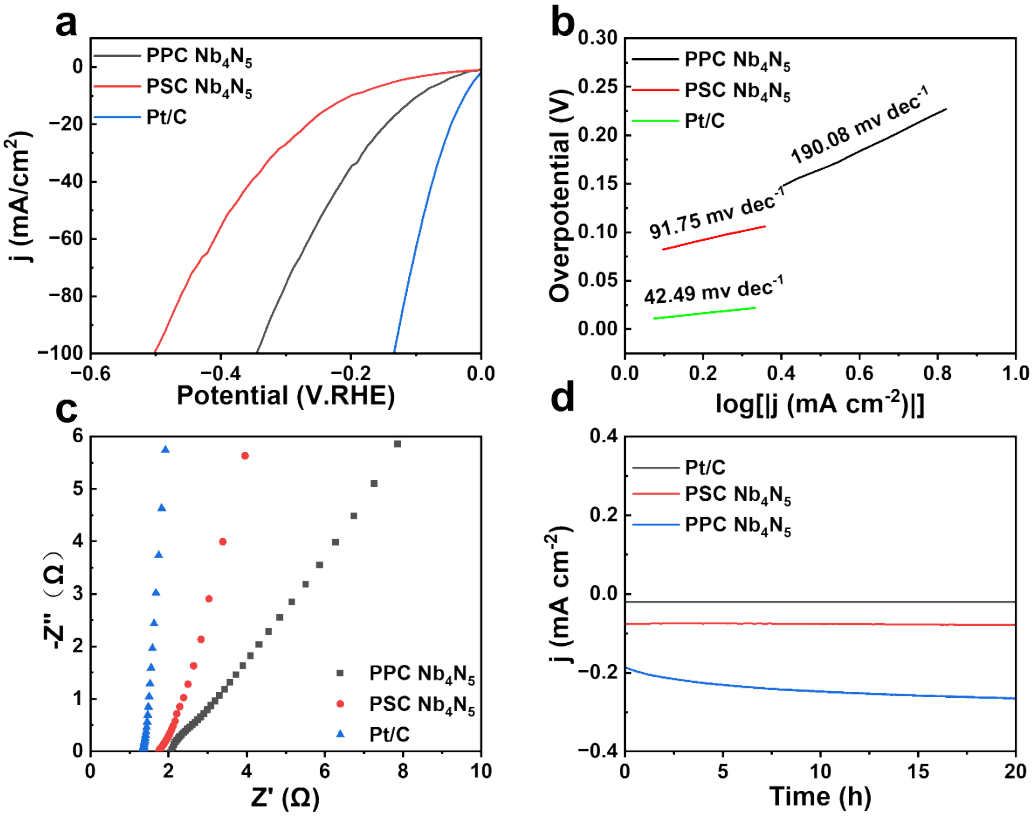


Fig. S6 (a) LSV curves of PSC Nb_4N_5, PPC Nb_4N_5 and Pt/C in 1 M KOH solution with a scan rate 5 mV s^{-1}. (b) Tafel slope of PSC Nb_4N_5, PPC Nb_4N_5 and Pt/C. (C) Nyquist plots of PSC Nb_4N_5, PPC Nb_4N_5 and Pt/C. (d) The durability test of PSC Nb_4N_5, PPC Nb_4N_5 and Pt/C for 20 h.

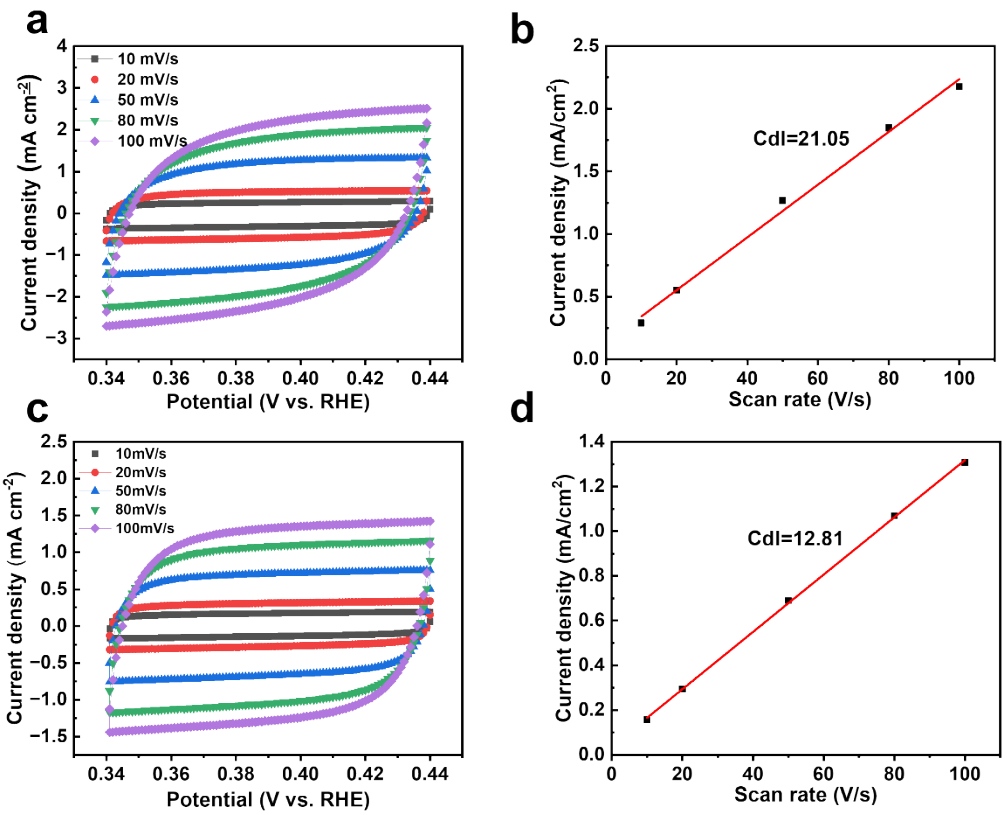


Fig. S7 CVs of (a) PSC Nb_4N_5 and (c) PPC Nb_4N_5 hexahedron catalysts at 10-100 mV s^{-1} in 0.5 M H_2SO_4 solution; (b) Plots providing the C_{dl} value of PSC Nb_4N_5 catalyst. (d) Plots providing the C_{dl} value of PPC Nb_4N_5 catalyst.

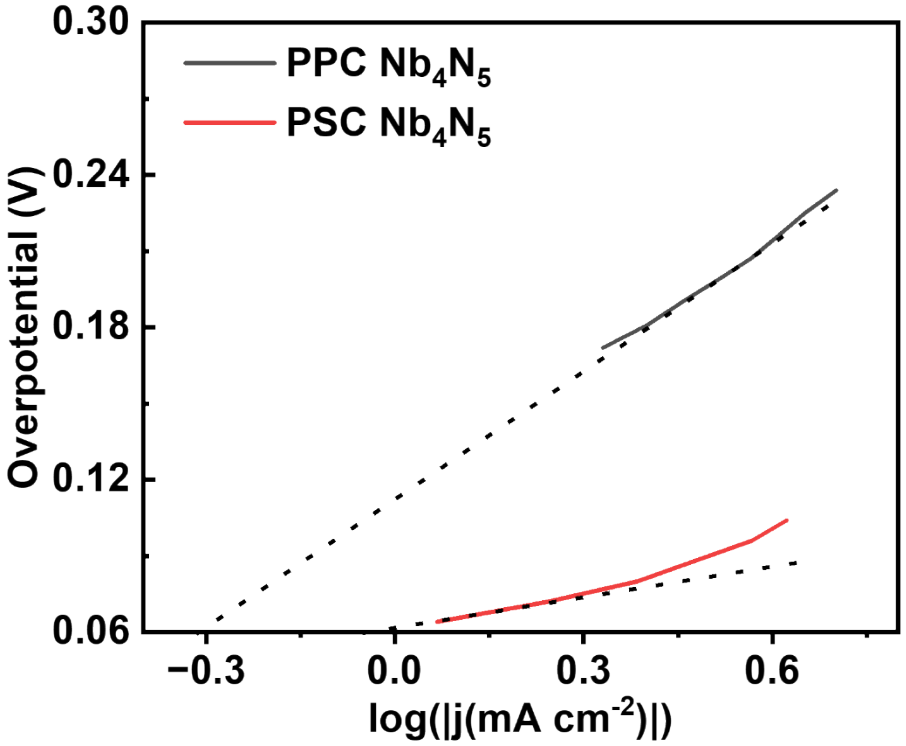


Fig. S8 Calculated exchange current densities of the PSC Nb_4N_5 and PPC Nb_4N_5 in 0.5 M H_2SO_4 electrolyte by applying extrapolation method to the Tafel plots.

Table S1. The comparison of HER electrocatalytic performance.

Catalyst	η(mV)at j=10mA cm^{-2}	Tafel slope	Electrolyte	references
PSC Nb_4N_5	71.86 mV	70.26 mV dec^{-1}	0.5 M H_2SO_4	This work
PPC Nb_4N_5	191.51 mV	169.02 mV dec^{-1}	0.5 M H_2SO_4	This work
Nb_2N	96.3 mV	92 mV dec^{-1}	0.5 M H_2SO_4	[1]
Sr_2RuO_4	61 mV	51 mV dec^{-1}	1 M KOH	[2]
Nb_4N_5−xOx/NG	39 mV	79 mV dec^{-1}	0.5 M H_2SO_4	[3]
PSC Mo_2N	73.13 mV	66.52 mV dec^{-1}	1 M KOH	[4]
PSC VN	74.67 mV	68.30 mV dec^{-1}	1 M KOH	[5]
Nb-Ti NNA	120 mV	52.90 mV dec^{-1}	1 M KOH	[6]
Co-NG	30 mV	82 mV dec^{-1}	0.5 M H_2SO_4	[7]
C-MoS_2	45 mV	46 mV dec^{-1}	1 M KOH	[8]
NiN	210 mV	122 mV dec^{-1}	1 M KOH	[9]

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