Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Porous single crystal niobium nitride and tantalum nitride nanocubes boost catalytic performance

Wanxiang Zhao,[a,b] Kui Xie [*b,c]

[a] College of Chemical Engineering, Fuzhou University, Fuzhou 350108, China.

[b] Key Laboratory of Design and Assembly of Functional Nanostructures, and Fujian Key Laboratory of Nanomaterials, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian 350002, China. E-mail: kxie@fjirsm.ac.cn.

[c] Advanced Energy Science and Technology Guangdong Laboratory, 29 Sanxin North Road, Huizhou, Guangdong 116023. China.

Lewis acid sites：

The density of Lewis acid sites at surface is calculated according to the equation:

$$d = D_{SAPO-34} \times A \times N_A / (A_{SAPO-34} \times S_{BET}) \quad (1)$$

Where d is the density of Lewis acid site of test samples, $D_{SAPO-34}$ is the density of acid site of standard sample SAPO-34 which is 2.55×10^{-4} mol/g.[1, 2] A is the integral area of the mass spectrometry signal of $-NH_2$ of PSC-N Ta_3N_5 or PSC-N Nb_4N_5 monoliths harvested by NH_3-TPD. $A_{SAPO-34}$ is the integral area of mass spectrometry signal of NH_3 of SAPO-34. N_A is the Avogadro's number. SBET is the specific surface area of PSC-N Ta_3N_5 or PSC-N Nb_4N_5.

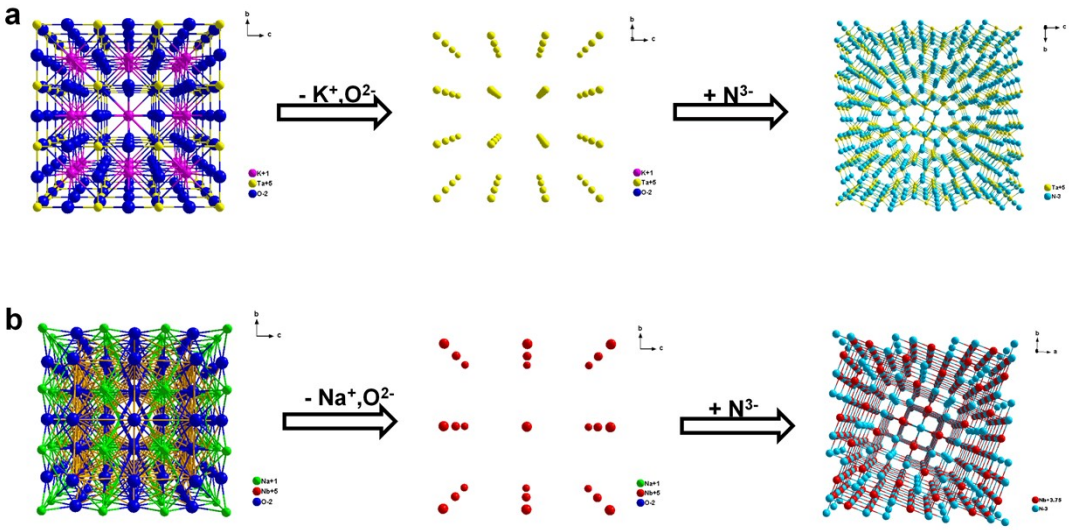

Fig. S1. Structure of $KTaO_3$ and $NaNbO_3$ Non-porous single crystal, and schematic procedure for the major experimental step of synthesis of PSC Nb_4N_5 and PSC Ta_3N_5.

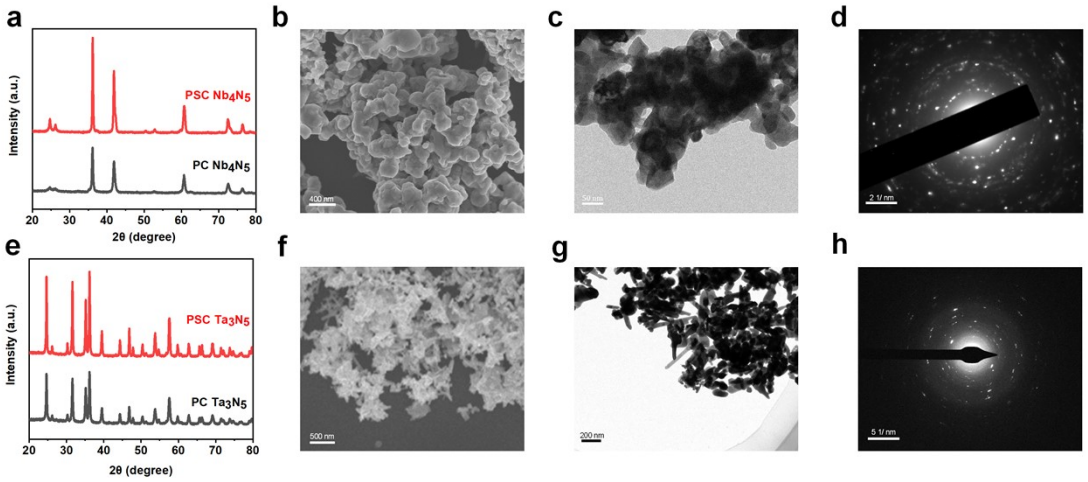

Fig. S2. (a-d) XRD pattern, SEM image, TEM image and SAED pattern of PC Nb_4N_5, respectively. (e-h) XRD pattern, SEM image, TEM image and SAED pattern of PC Ta_3N_5, respectively.

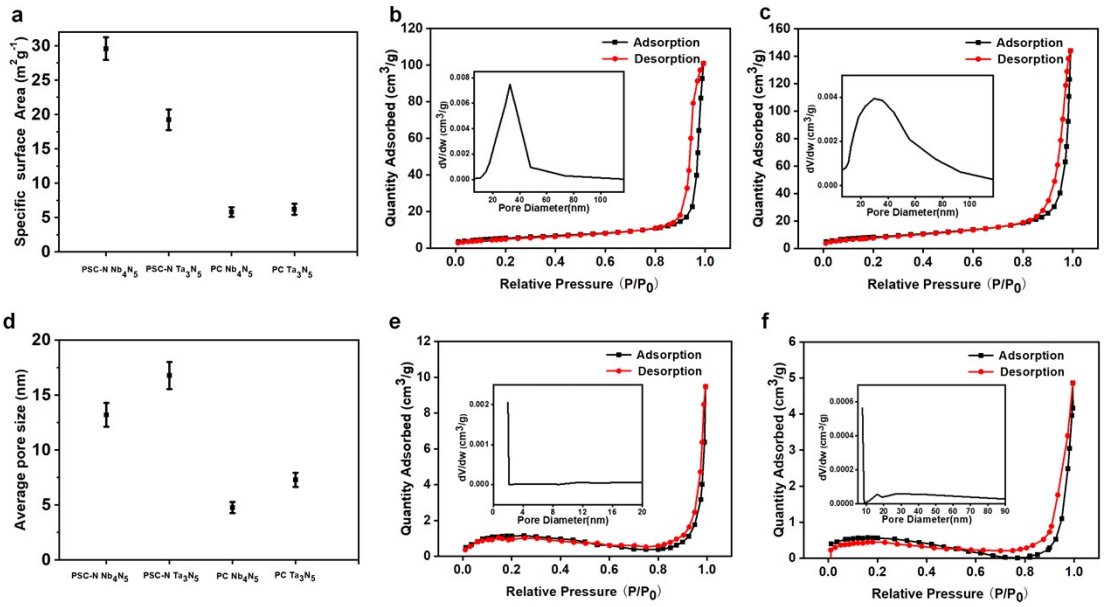

Fig. S3. (a, d) The Specific surface area and average pore size of PSC-N Nb_4N_5, Ta_3N_5 and PC Nb_4N_5, Ta_3N_5. (b) Nitrogen adsorption-desorption isotherm of PSC-N Nb_4N_5. (c) Nitrogen adsorption-desorption isotherm of PSC-N Ta_3N_5. (e) Nitrogen adsorption-desorption isotherm of PC Nb_4N_5. (f) Nitrogen adsorption-desorption isotherm of PC Ta_3N_5.

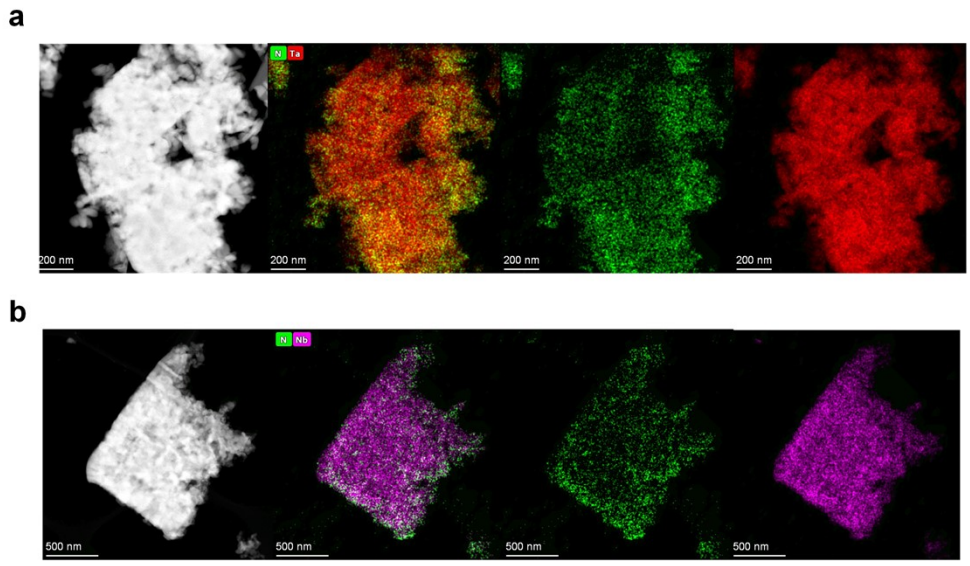

Fig. S4. TEM mapping images of Ta_3N_5 and Nb_4N_5

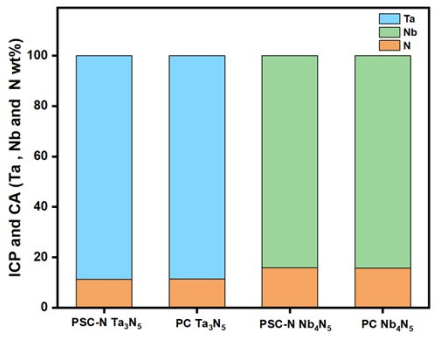

Fig. S5. The element analysis of Ta_3N_5 and Nb_4N_5

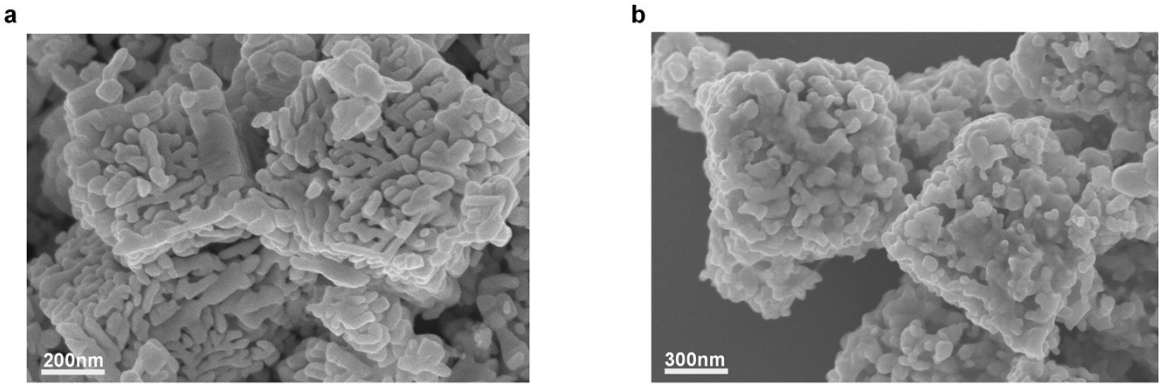

Fig. S6. (a) PSC-N Ta_3N_5 (b) PSC-N Nb_4N_5.

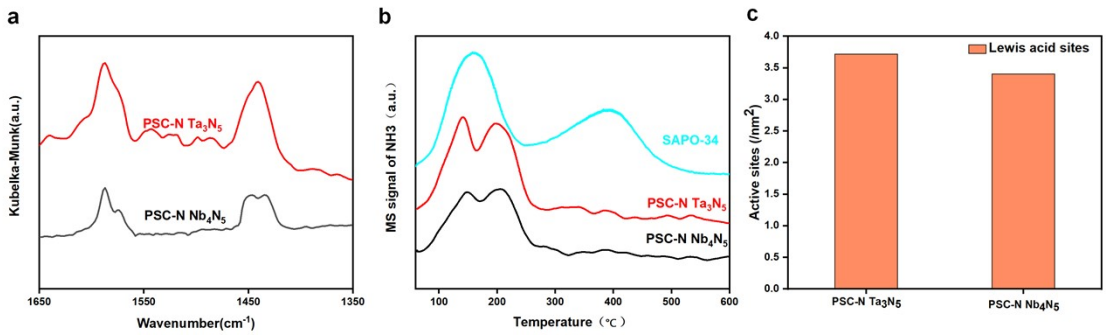

Figure.S7. (a) FTIR spectra of adsorbed pyridine (b) NH_3-TPD profiles of PSC-N Ta_3N_5, PSC-N Nb_4N_5 and molecular sieves sample (SAPO-34) (c) Density of Lewis acid sites of different catalysts

Table S1. Comparative performance of ethane dehydrogenation to ethylene for PSC-N Ta_3N_5 and PSC-N Nb_4N_5 with other catalysts

Catalyst	Temperature (℃)	Gas composition	C_2H_6 conversion & C_2H_4 selectivity (%)		Ref
PSC-N Ta_3N_5	**680**	**C_2H_6/He=1:9**	**23.6%**	**92.4%**	**This work**
PSC-N Nb_4N_5	**680**	**C_2H_6/He=1:9**	**21.4%**	**90%**	**This work**
Pt@HZSM-5	550	C_2H_6/N_2=9:1	15.2%	88.4%	3
MoN	660	C_2H_6/He=1:9	25%	99%	4
2.5 wt.% P+ Mo/ZSM5	600	C_2H_4/N_2/He=1:1:8	17%	77%	5
Pt/M-TS-1	600	C_2H_6/Ar =3:1	15.7%	99%	6
$CsRu/CeO_2$	700	C_2H_6/N_2=1:1	41%	87%	7
0.8Cr/MFI	650	C_2H_6/N_2=2:8	17.2%	99%	8
0.125-Pd /TiO_2	Room temperature	C_2H_6/Ar =1:1	0.26%	94.2%	9

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