

Supporting information

Mixed $\text{NaNb}_x\text{Ta}_{1-x}\text{O}_3$ perovskites as photocatalysts for H_2 production

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Table S1: Elemental analysis of the prepared samples from ICP-AES technique

Sample Name	Synthesis method	Observed wt % of the element [] ^a			
		Na	Ta	Nb	Pt ^b
NaTaO ₃	SSR	8.2 ± 0.3 [9.1]	75.5 ± 1.5 [71.8]	--	--
NaNb _{0.25} Ta _{0.75} O ₃	SSR	9.3 ± 0.3 [10.0]	62.2 ± 1.2 [59.0]	9.9 ± 0.3 [10.1]	--
NaNb _{0.5} Ta _{0.5} O ₃	SSR	10.3 ± 0.3 [11.1]	46.8 ± 0.9 [43.5]	22.7 ± 0.5 [22.3]	0.11 ± 0.01 [0.125] 0.48 ± 0.01 [0.5]
NaNb _{0.75} Ta _{0.25} O ₃	SSR	11.5 ± 0.3 [12.4]	24.8 ± 0.5 [24.3]	38.2 ± 0.8 [37.5]	--
NaNbO ₃	SSR	13.2 ± 0.4 [14.0]	--	59.0 ± 1.2 [56.7]	--
NaNb _{0.5} Ta _{0.5} O ₃	Hyd	10.6 ± 0.3 [11.1]	46.7 ± 0.9 [43.5]	22.9 ± 0.5 [22.3]	0.12 ± 0.01 [0.125] 0.52 ± 0.02 [0.5]

^aNominal value is indicated in the parenthesis.

^bPt loading over the sample measured after reaction.

Figure S1: SEM and EDS element mapping of $\text{NaNb}_x\text{Ta}_{1-x}\text{O}_3$ samples

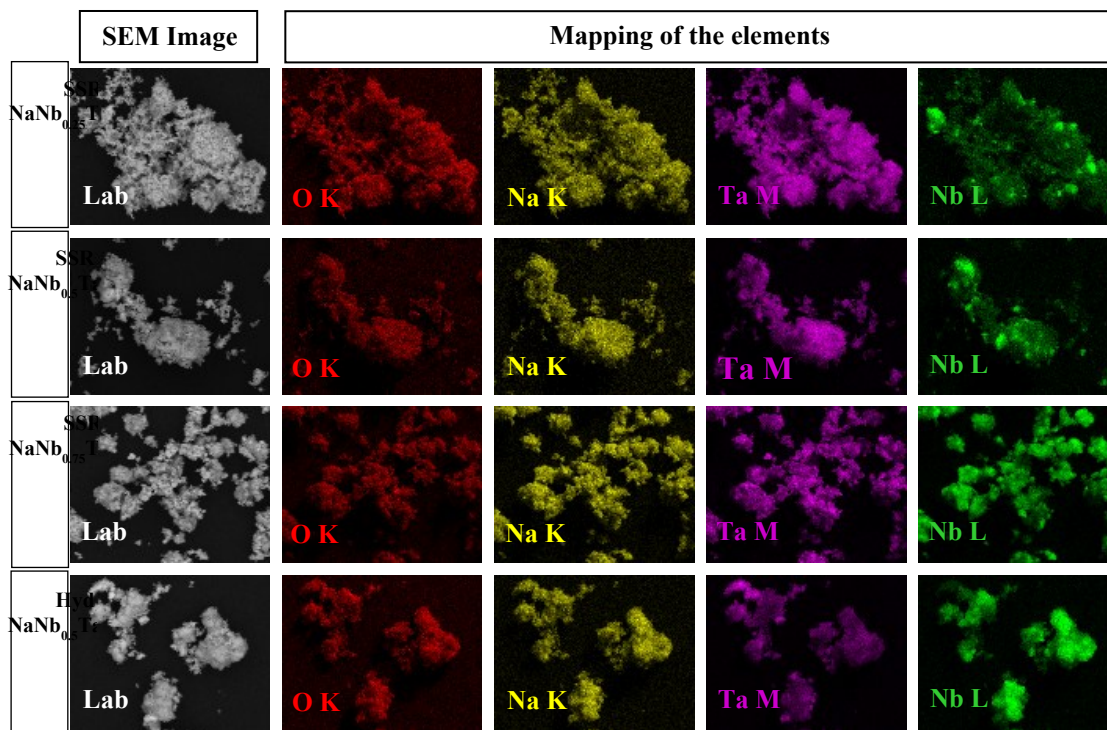
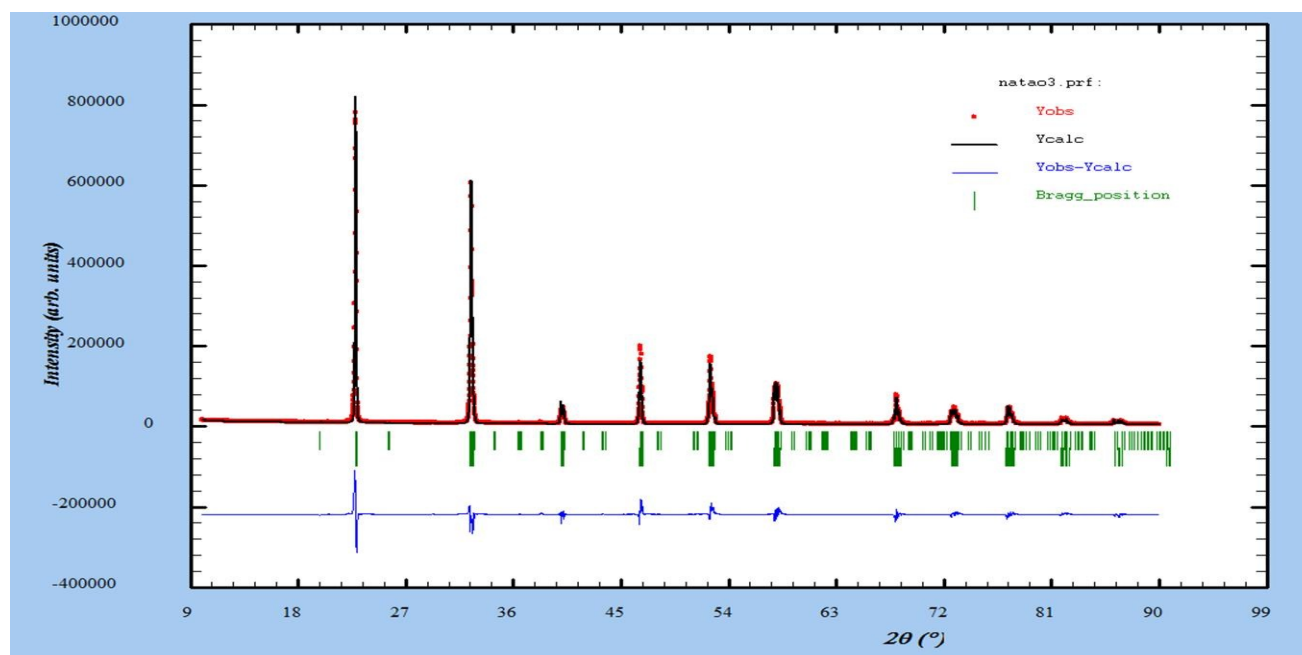


Figure S2: Rietveld analysis of the observed XRD pattern of NaTaO₃ by using Fullprof Suite.



Analysis results

=> Phase No. 1 NaTaO₃ Pcmn P c m n

=> Atom Parameters:

Name	x	sx	y	sy	z	sz	B	sB	occ.	socc.	Mult
O1	0.21490(0)		0.02950(0)		0.28400(0)		0.500(0)		1.000(0)		8
O2	0.43810(0)		0.25000(0)		0.00920(0)		0.500(0)		1.000(0)		4
NA1	0.99530(0)		0.25000(0)		0.98420(0)		0.500(0)		1.000(0)		4
TA1	0.50000(0)		0.00000(0)		0.00000(0)		0.500(0)		1.000(0)		4

=> Cell parameters: a: 5.47949 b: 7.79260 c: 5.52570 α=β=γ=90.0000

=> Phase No. 2 NaTaO₃ P12m1 P 1 2/m 1

=> Atom Parameters:

Name	x	sx	y	sy	z	sz	B	sB	occ.	socc.	Mult
O1	0.50000(0)		0.50000(0)		0.00000(0)		0.500(0)		1.000(0)		1
O2	0.00000(0)		0.50000(0)		0.50000(0)		0.500(0)		1.000(0)		1
O3	0.50000(0)		0.00000(0)		0.50000(0)		0.500(0)		1.000(0)		1
TA1	0.50000(0)		0.50000(0)		0.50000(0)		0.500(0)		1.000(0)		1
NA1	0.00000(0)		0.00000(0)		0.00000(0)		0.500(0)		1.000(0)		1

=> Cell parameters: a: 3.88926 b: 3.89602 c: 3.90119 α=γ=90.0000 β= 90.28562

BRAGG R-Factors and weight fractions for Pattern # 1

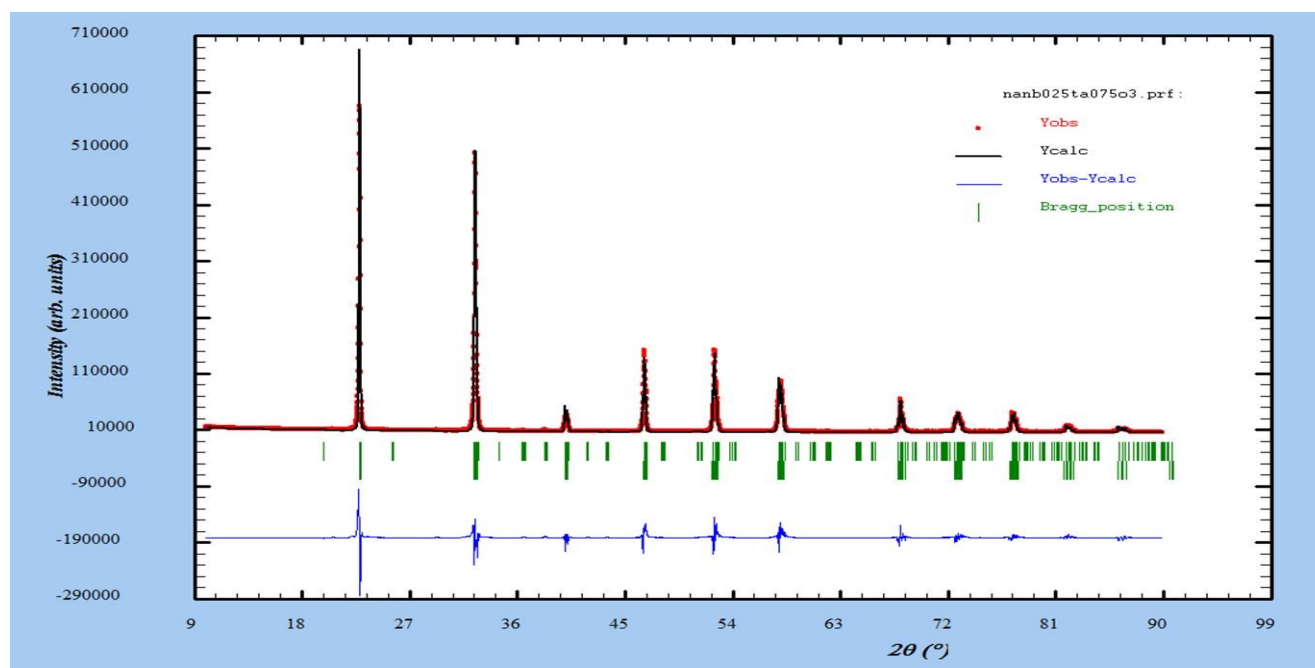
=> Phase: 1 NaTaO₃ Pcmn

=> Bragg R-factor: 18.5 Vol: 235.944(0.011) Fract(%): **35.50**(0.89)
=> Rf-factor= 31.9 ATZ: 1887.492 Brindley: 1.0000

=> Phase: 2 NaTaO₃ P12m1

=> Bragg R-factor: 10.2 Vol: 59.113(0.004) Fract(%): **64.50**(1.77)
=> Rf-factor= 6.04 ATZ: 4030.974 Brindley: 1.0000

Figure S3: Rietveld analysis of the observed XRD pattern of $\text{NaNb}_{0.25}\text{Ta}_{0.75}\text{O}_3$ by using Fullprof Suite.



Analysis results

=> Phase No. 1 NaTaO_3 Pcmn P c m n

=> Atom Parameters:

Name	x	sx	y	sy	z	sz	B	sB	occ.	socc.	Mult
O1	0.21490(0)		0.02950(0)		0.28400(0)		0.500(0)		1.000(0)		8
O2	0.43810(0)		0.25000(0)		0.00920(0)		0.500(0)		1.000(0)		4
NA1	0.99530(0)		0.25000(0)		0.98420(0)		0.500(0)		1.000(0)		4
TA1	0.50000(0)		0.00000(0)		0.00000(0)		0.500(0)		1.000(0)		4

=> Cell parameters: a: 5.48141 b: 7.79029 c: 5.52392 $\alpha=\beta=\gamma=90.0000$

=> Phase No. 2 NaTaO_3 P12m1 P 1 2/m 1

=> Atom Parameters:

Name	x	sx	y	sy	z	sz	B	sB	occ.	socc.	Mult
O1	0.50000(0)		0.50000(0)		0.00000(0)		0.500(0)		1.000(0)		1
O2	0.00000(0)		0.50000(0)		0.50000(0)		0.500(0)		1.000(0)		1
O3	0.50000(0)		0.00000(0)		0.50000(0)		0.500(0)		1.000(0)		1
TA1	0.50000(0)		0.50000(0)		0.50000(0)		0.500(0)		1.000(0)		1
NA1	0.00000(0)		0.00000(0)		0.00000(0)		0.500(0)		1.000(0)		1

=> Cell parameters: a: 3.90357 b: 3.89687 c: 3.89038 $\alpha=\gamma=90.0000$ $\beta=90.31082$

BRAGG R-Factors and weight fractions for Pattern # 1

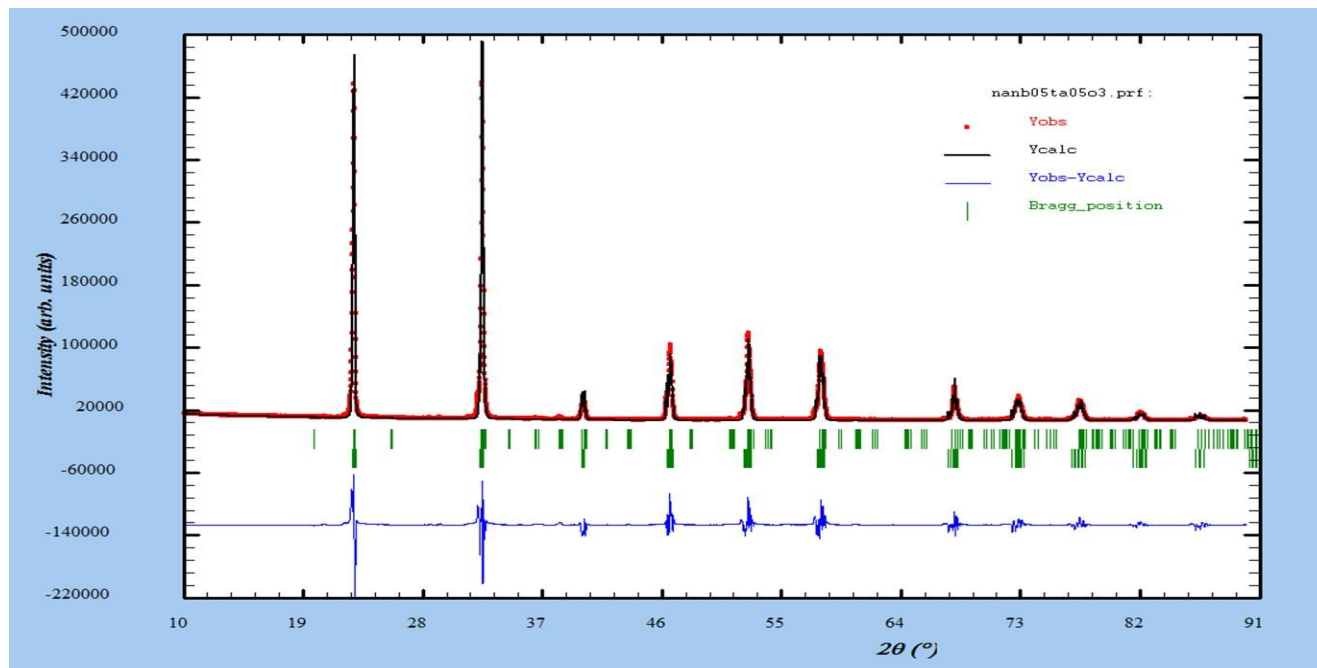
=> Phase: 1 NaTaO_3 Pcmn

=> Bragg R-factor: 18.3 Vol: 235.881(0.000) Fract(%): **29.11**(0.71)
=> Rf-factor= 31.7 ATZ: 1887.492 Brindley: 1.0000

=> Phase: 2 NaTaO_3 P12m1

=> Bragg R-factor: 10.6 Vol: 59.178(0.003) Fract(%): **70.89**(1.57)
=> Rf-factor= 6.80 ATZ: 4030.974 Brindley: 1.0000

Figure S4: Rietveld analysis of the observed XRD pattern of $\text{NaNb}_{0.5}\text{Ta}_{0.5}\text{O}_3$ by using Fullprof Suite.



Analysis results

=> Phase No. 1 NaTaO_3 Pcmn P c m n

=> Atom Parameters:

Name	x	sx	y	sy	z	sz	B	sB	occ.	socc.	Mult
O1	0.21490(0)	0.02950(0)	0.28400(0)	0.500(0)	1.000(0)	8					
O2	0.43810(0)	0.25000(0)	0.00920(0)	0.500(0)	1.000(0)	4					
NA1	0.99530(0)	0.25000(0)	0.98420(0)	0.500(0)	1.000(0)	4					
TA1	0.50000(0)	0.00000(0)	0.00000(0)	0.500(0)	1.000(0)	4					

=> Cell parameters: a: 5.48114 b: 7.78872 c: 5.52062 $\alpha=\beta=\gamma=90.0000$

=> Phase No. 2 NaTaO_3 P12m1 P 1 2/m 1

=> Atom Parameters:

Name	x	sx	y	sy	z	sz	B	sB	occ.	socc.	Mult
O1	0.50000(0)	0	0.50000(0)	0	0.00000(0)	0	0.500(0)	1.000(0)	1		
O2	0.00000(0)	0	0.50000(0)	0	0.50000(0)	0	0.500(0)	1.000(0)	1		
O3	0.50000(0)	0	0.00000(0)	0	0.50000(0)	0	0.500(0)	1.000(0)	1		
TA1	0.50000(0)	0	0.50000(0)	0	0.50000(0)	0	0.500(0)	1.000(0)	1		
NA1	0.00000(0)	0	0.00000(0)	0	0.00000(0)	0	0.500(0)	1.000(0)	1		

=> Cell parameters: a: 3.91412 b: 3.88426 c: 3.90105 $\alpha=\gamma=90.0000$ $\beta=90.30182$

BRAGG R-Factors and weight fractions for Pattern # 1

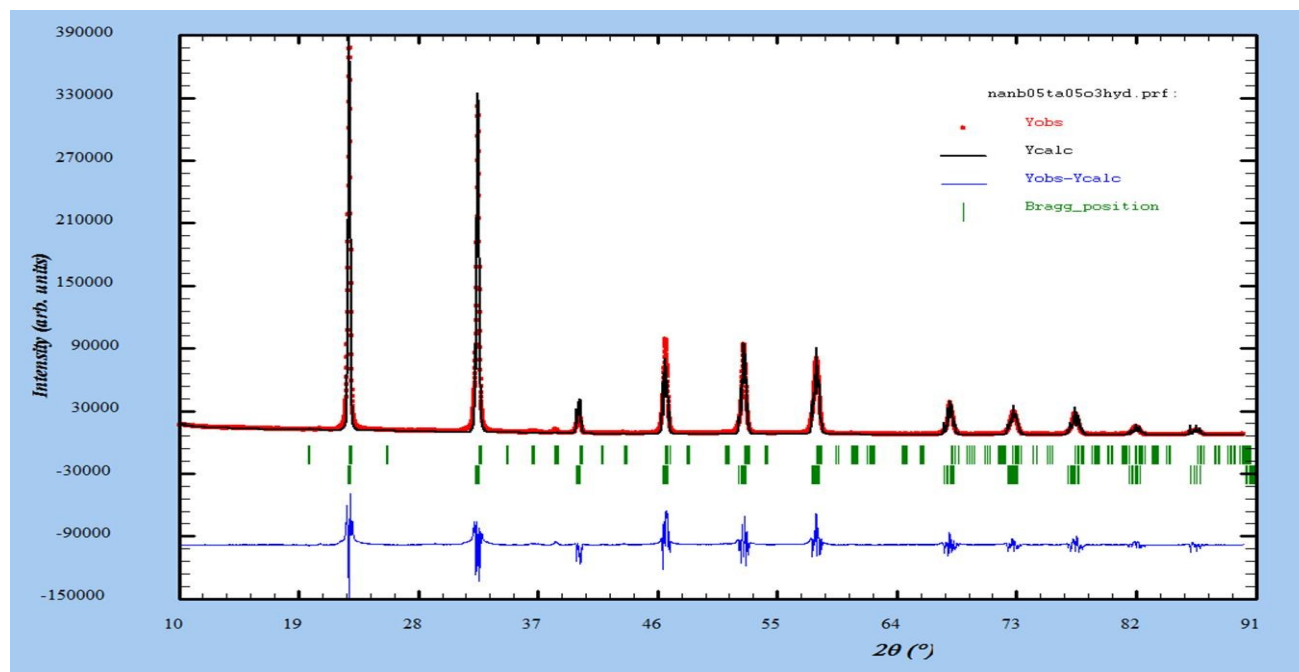
=> Phase: 1 NaTaO_3 Pcmn

=> Bragg R-factor: 18.0 Vol: 235.681(0.000) Fract(%): **25.61**(0.46)
=> Rf-factor= 29.1 ATZ: 1887.492 Brindley: 1.0000

=> Phase: 2 NaTaO_3 P12m1

=> Bragg R-factor: 13.2 Vol: 59.309(0.003) Fract(%): **74.39**(1.12)
=> Rf-factor= 7.31 ATZ: 4030.974 Brindley: 1.0000

Figure S5: Rietveld analysis of the observed XRD pattern of Hyd-NaNb_{0.5}Ta_{0.5}O₃ by using Fullprof Suite.



Analysis results

=> Phase No. 1 NaTaO₃ Pcmn P c m n

=> Atom Parameters:

Name	x	sx	y	sy	z	sz	B	sB	occ.	socc.	Mult
O1	0.21490(0)	0.02950(0)	0.28400(0)	0.500(0)	1.000(0)	8					
O2	0.43810(0)	0.25000(0)	0.00920(0)	0.500(0)	1.000(0)	4					
NA1	0.99530(0)	0.25000(0)	0.98420(0)	0.500(0)	1.000(0)	4					
TA1	0.50000(0)	0.00000(0)	0.00000(0)	0.500(0)	1.000(0)	4					

=> Cell parameters: a: 5.49600 b: 7.79639 c: 5.48250 $\alpha=\beta=\gamma=90.0000$

=> Phase No. 2 NaTaO₃ P12m1 P 1 2/m 1

=> Atom Parameters:

Name	x	sx	y	sy	z	sz	B	sB	occ.	socc.	Mult
O1	0.50000(0)	0	0.50000(0)	0	0.00000(0)	0	0.500(0)	1.000(0)	1		
O2	0.00000(0)	0	0.50000(0)	0	0.50000(0)	0	0.500(0)	1.000(0)	1		
O3	0.50000(0)	0	0.00000(0)	0	0.50000(0)	0	0.500(0)	1.000(0)	1		
TA1	0.50000(0)	0	0.50000(0)	0	0.50000(0)	0	0.500(0)	1.000(0)	1		
NA1	0.00000(0)	0	0.00000(0)	0	0.00000(0)	0	0.500(0)	1.000(0)	1		

=> Cell parameters: a: 3.91344 b: 3.89408 c: 3.90027 $\alpha=\gamma=90.0000$ $\beta=90.35083$

BRAGG R-Factors and weight fractions for Pattern # 1

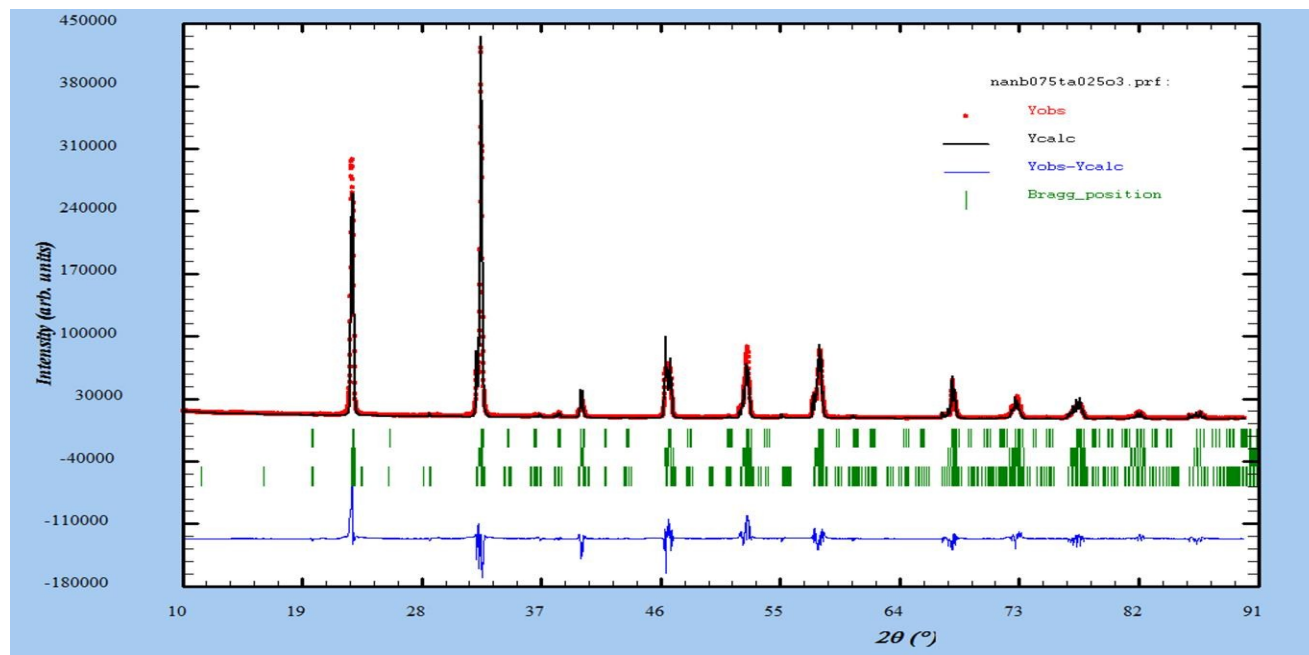
=> Phase: 1 NaTaO₃ Pcmn

=> Bragg R-factor: 22.4 Vol: 234.919(0.017) Fract(%): **18.78**(0.30)
=> Rf-factor= 33.1 ATZ: 1887.492 Brindley: 1.0000

=> Phase: 2 NaTaO₃ P12m1

=> Bragg R-factor: 12.0 Vol: 59.436(0.003) Fract(%): **81.22**(0.88)
=> Rf-factor= 7.45 ATZ: 4030.974 Brindley: 1.0000

Figure S6: Rietveld analysis of the observed XRD pattern of $\text{NaNb}_{0.75}\text{Ta}_{0.25}\text{O}_3$ by using Fullprof Suite.



Analysis results

=> Phase No. 1 NaTaO_3 Pcmn P c m n

=> Atom Parameters:

Name	x	sx	y	sy	z	sz	B	sB	occ.	socc.	Mult
O1	0.21490(0)	0.02950(0)	0.28400(0)	0.500(0)	0.500(0)	0.500(0)	1.000(0)	1.000(0)	8		
O2	0.43810(0)	0.25000(0)	0.00920(0)	0.500(0)	0.500(0)	0.500(0)	1.000(0)	1.000(0)	4		
NA1	0.99530(0)	0.25000(0)	0.98420(0)	0.500(0)	0.500(0)	0.500(0)	1.000(0)	1.000(0)	4		
TA1	0.50000(0)	0.00000(0)	0.00000(0)	0.500(0)	0.500(0)	0.500(0)	1.000(0)	1.000(0)	4		

=> Cell parameters: a: 5.49252 b: 7.79922 c: 5.51565 $\alpha=\beta=\gamma=90.0000$

=> Phase No. 2 NaTaO_3 P12m1 P 1 2/m 1

=> Atom Parameters:

Name	x	sx	y	sy	z	sz	B	sB	occ.	socc.	Mult
O1	0.50000(0)		0.50000(0)		0.00000(0)		0.500(0)		1.000(0)		1
O2	0.00000(0)		0.50000(0)		0.50000(0)		0.500(0)		1.000(0)		1
O3	0.50000(0)		0.00000(0)		0.50000(0)		0.500(0)		1.000(0)		1
TA1	0.50000(0)		0.50000(0)		0.50000(0)		0.500(0)		1.000(0)		1
NA1	0.00000(0)		0.00000(0)		0.00000(0)		0.500(0)		1.000(0)		1

=> Cell parameters: a: 3.92134 b: 3.90748 c: 3.88127 $\alpha=\gamma=90.0000$ $\beta=90.12099$

=> Phase No. 3 NaNbO_3 Pbcm P b c m

=> Atom Parameters:

Name	x	sx	y	sy	z	sz	B	sB	occ.	socc.	Mult
NA1	0.23900(0)	0.78200(0)	0.25000(0)	0.500(0)	0.500(0)	0.500(0)	1.000(0)	1.000(0)	4		
NA2	0.24300(0)	0.75000(0)	0.00000(0)	0.500(0)	0.500(0)	0.500(0)	1.000(0)	1.000(0)	4		
O1	0.96600(0)	0.46700(0)	0.11000(0)	0.500(0)	0.500(0)	0.500(0)	1.000(0)	1.000(0)	8		
O2	0.53600(0)	0.03200(0)	0.14000(0)	0.500(0)	0.500(0)	0.500(0)	1.000(0)	1.000(0)	8		
O3	0.19100(0)	0.23300(0)	0.25000(0)	0.500(0)	0.500(0)	0.500(0)	1.000(0)	1.000(0)	4		
O4	0.30400(0)	0.25000(0)	0.00000(0)	0.500(0)	0.500(0)	0.500(0)	1.000(0)	1.000(0)	4		

NB1 0.25660(0) 0.27220(0) 0.12620(0) 0.500(0) 1.000(0) 8

=> Cell parameters: a: 5.50089 b: 5.56728 c: 15.53942 $\alpha=\beta=\gamma=90.0000$

BRAGG R-Factors and weight fractions for Pattern # 1

=> Phase: 1 NaTaO₃ Pcmn

=> Bragg R-factor: 15.3 Vol: 236.276(0.015) Fract(%): **8.20**(0.08)

=> Rf-factor= 18.5 ATZ: 1887.492 Brindley: 1.0000

=> Phase: 2 NaTaO₃ P12m1

=> Bragg R-factor: 16.9 Vol: 59.471(0.004) Fract(%): **16.21**(0.30)

=> Rf-factor= 10.3 ATZ: 4030.974 Brindley: 1.0000

=> Phase: 3 NaNbO₃ Pbcm

=> Bragg R-factor: 26.0 Vol: 475.894(0.022) Fract(%): 75.59(1.24)

=> Rf-factor= 32.3 ATZ: 3246.137 Brindley: 1.0000

Figure S7: The activity comparison of high performance Hyd-NaNb_{0.5}Ta_{0.5}O₃ catalyst with 1:1 physical mixture of NaTaO₃ and NaNbO₃ samples in presence of 0.5 wt% of Pt.

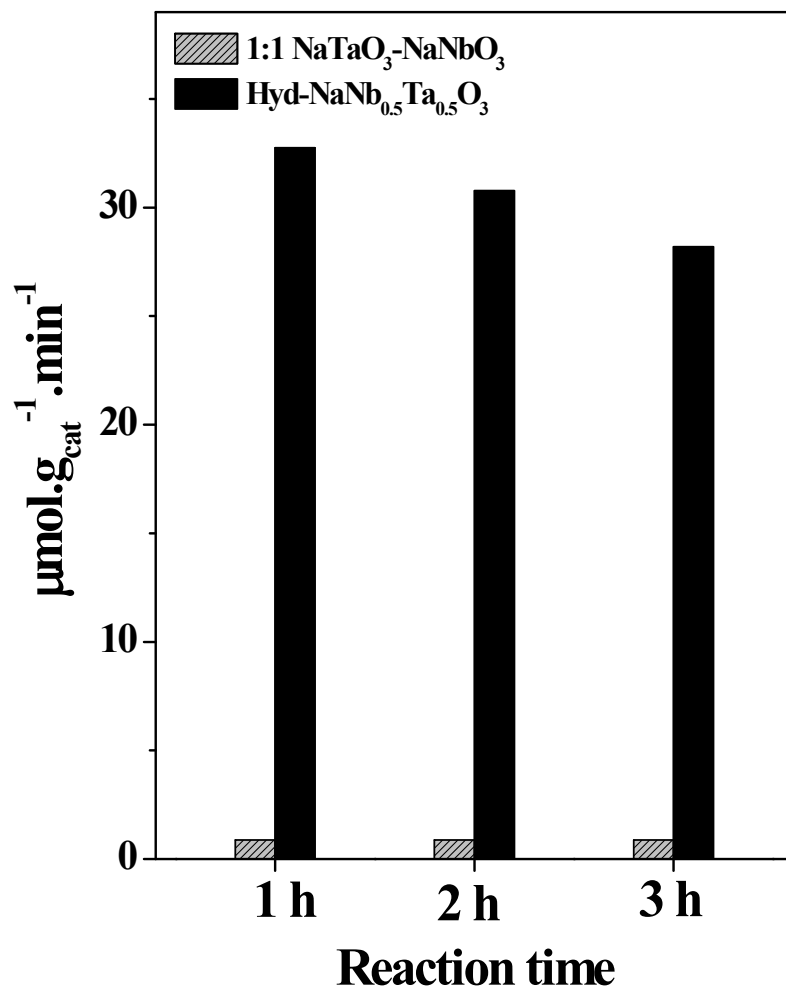


Figure S8: The H₂ production activity of the catalyst after 6h of reaction with various loadings of Pt.

