

## Influence of calcination on performance of Bi-Ni-O/gamma-alumina catalyst for *n*-butane oxidative dehydrogenation to butadiene

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Supporting data:

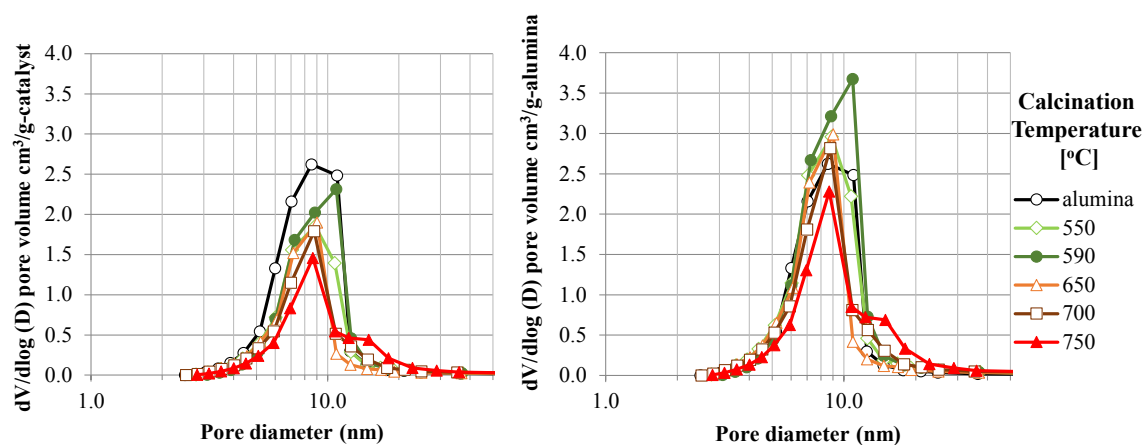


Fig. s1 Pore size distribution of catalysts with calcination temperature

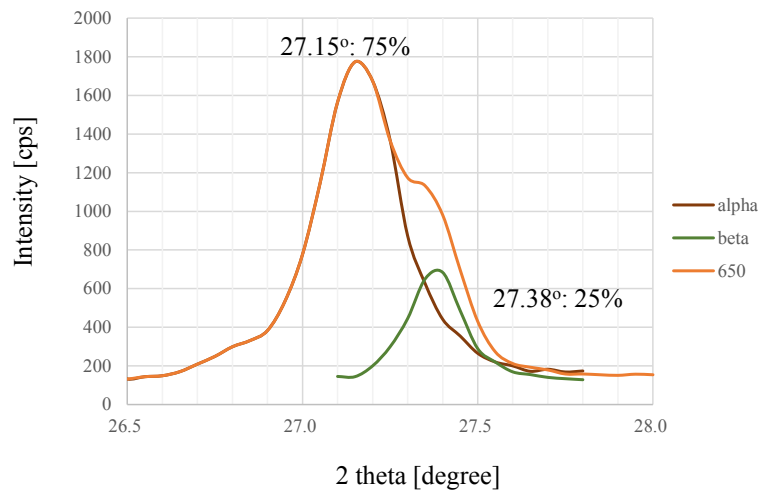


Fig.s2. XRD peak deconvolution of catalyst calcined at 650 °C

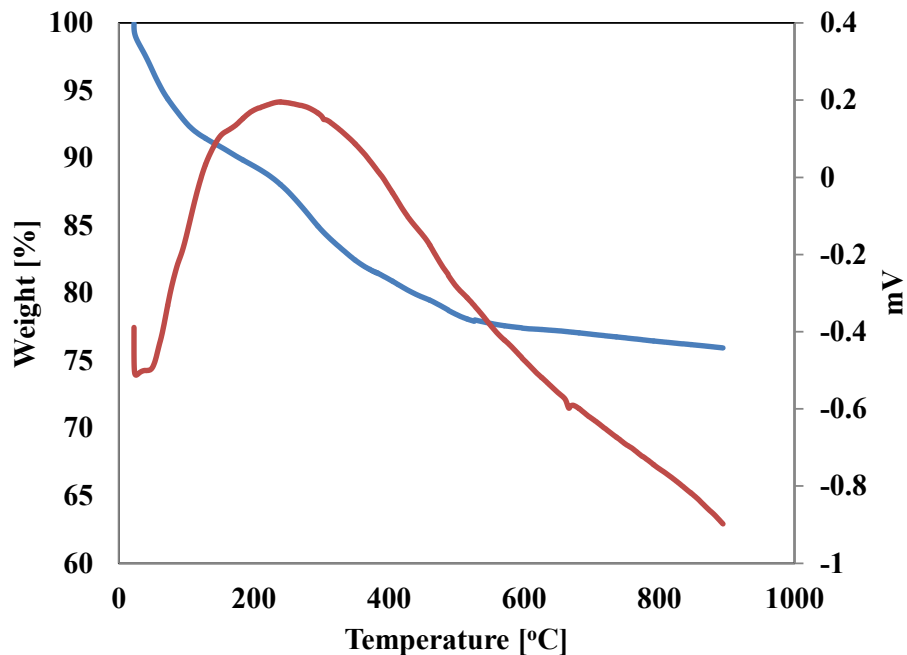


Fig. s3 TGA-DTA analysis for as-synthesized standard sample 30wt%Bi-20wt%Ni-O/Al<sub>2</sub>O<sub>3</sub>.

TGA-DTA analysis was carried out for as-synthesized standard sample 30wt%Bi-20wt%Ni-O/Al<sub>2</sub>O<sub>3</sub>. The TGA showed main weight loss occur at 250 - 350 °C (17%), and the second weight loss extends until 510 °C (5%). On the other hand, in DTA analysis, the structure change detected by XRD was not clearly observed.

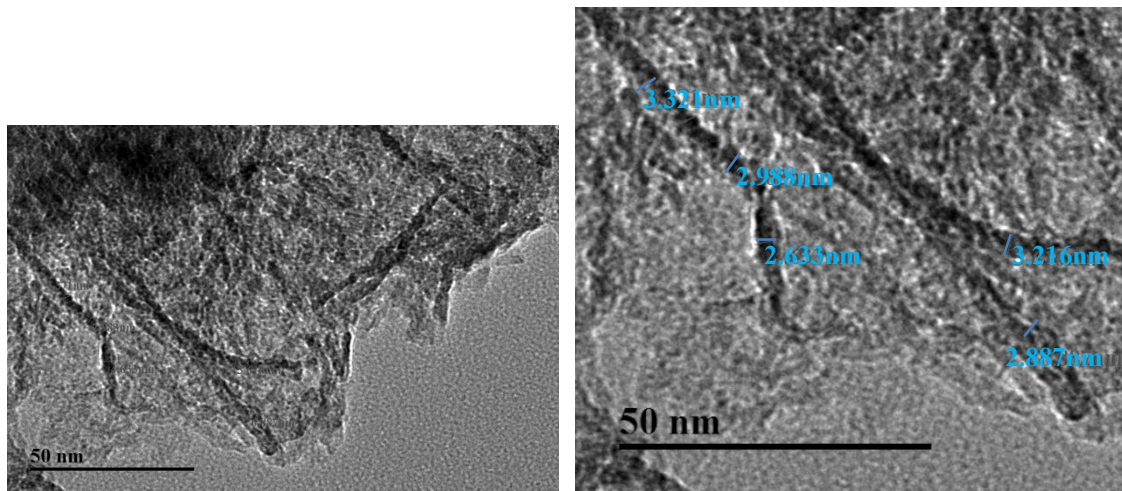


Fig. s4 TEM images of 20wt%Ni-O/Al<sub>2</sub>O<sub>3</sub> catalyst (Right: for NiO size measurement)

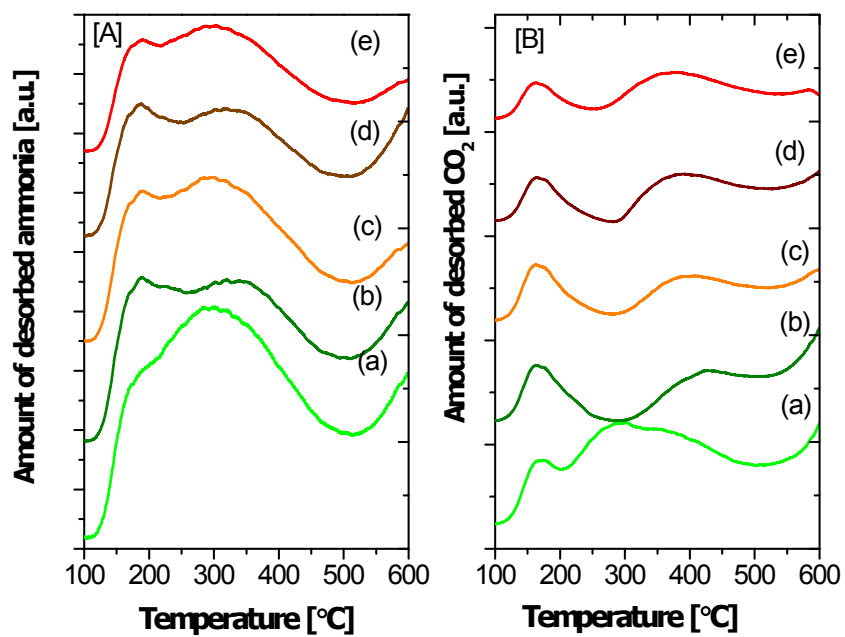


Fig. s5 TPD profile (NH<sub>3</sub> & CO<sub>2</sub>) with various calcination temperatures, (a) 550 °C, (b) 590 °C, (c) 650 °C, (d) 700 °C and (e) 750 °C.

The products found in GC with selectivity for one step and two step sample of Table 1 of manuscript is provided as supplementary table 'Table s1'.

Table s1 Products found in GC with selectivity for one step and two step sample of Table 1.

Reaction temp. [°C]	400		400		450	
O <sub>2</sub> /n-C <sub>4</sub> H <sub>10</sub> [mol/mol]	1		2		2	
Calcination step <sup>a</sup>	one	two	one	two	one	two
n-C <sub>4</sub> H <sub>10</sub> conversion [%]	11.8	14.1	18.4	18.3	25.9	26.9
DH selec	66.9	79.8	58.7	77.5	54.3	74.8
1-C <sub>4</sub> <sup>=</sup>	19.5	19.0	16.5	19.9	11.3	14.8
t-2-C <sub>4</sub> <sup>=</sup>	20.7	17.4	17.0	15.2	14.1	12.0
c-2-C <sub>4</sub> <sup>=</sup>	17.6	14.6	15.0	13.4	10.9	9.0
BD	9.1	28.8	10.2	29.0	18.0	39.0
OC selec	30.0	19.3	38.2	21.1	43.9	24.1
Ox	23.0	18.1	27.1	19.4	18.7	16.3
C <sub>3</sub> <sup>=</sup>	3.0	0.3	4.1	0.3	6.8	1.3
C <sub>2</sub> <sup>=</sup>	4.0	0.9	6.3	1.4	15.4	6.5
C <sub>3</sub>	0.0	0.0	0.0	0.0	0.3	0.0
C <sub>2</sub>	0.0	0.0	0.0	0.0	0.3	0.0
C <sub>1</sub>	0.0	0.0	0.7	0.0	2.5	0.0
PO selec (CO)	3.0	0.8	3.2	1.3	1.8	1.1
S <sub>sum</sub>	100.0	100.0	100.0	100.0	100.0	100.0

<sup>a</sup>one step: 590 °C-2h, two step: 350 °C-1h+590 °C-2h

<sup>b</sup> DH: dehydrogenation, BD: butadiene, OC: oxygenate and the cracked, PO: partial oxidation.

Table s2. H<sub>2</sub> consumption in TPR of 30wt%Bi-20wt%Ni-O/Al<sub>2</sub>O<sub>3</sub> catalysts calcined at various temperatures.

Calcination Temperature (°C)	TPR				
	H <sub>2</sub> consumption [m mol/g] ( T <sub>M</sub> [°C])				
	I	II	III	IV	total
550	1.09 (500)	1.59 (600)	2.66 (680)	0.26 (850)	5.60
590	0.45 (500)	1.15 (600)	3.18 (700)	0.12 (850)	4.90
650	2.54 (500)	3.43 (650)	-	1.16(850)	7.13
700	2.30 (500)	3.40(630)	-	1.32 (860)	7.02
750	1.86 (500)	3.62 (620)	-	1.11 (870)	6.59