Supplementary material

Catalytic performance of ternary Mg-Al-Ce oxides for ethanol conversion into 1-butanol in a flow reactor

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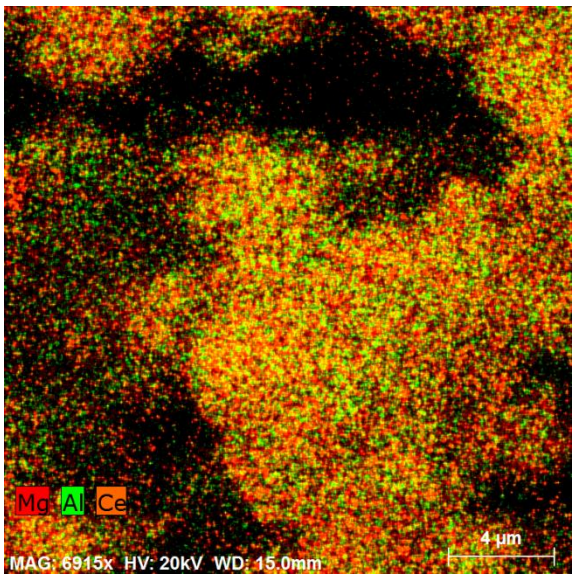
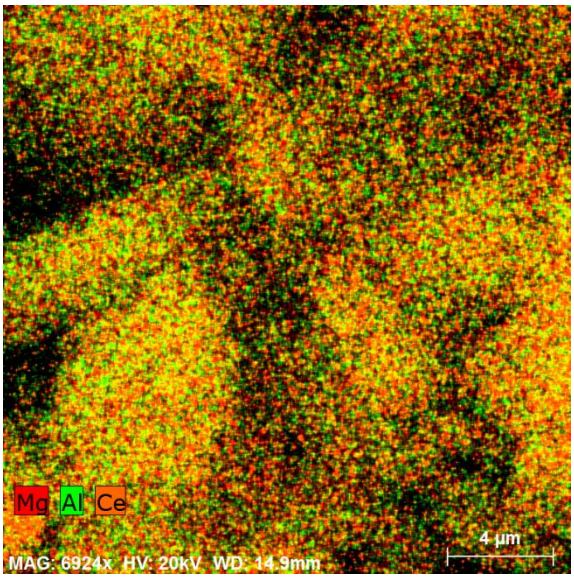


A



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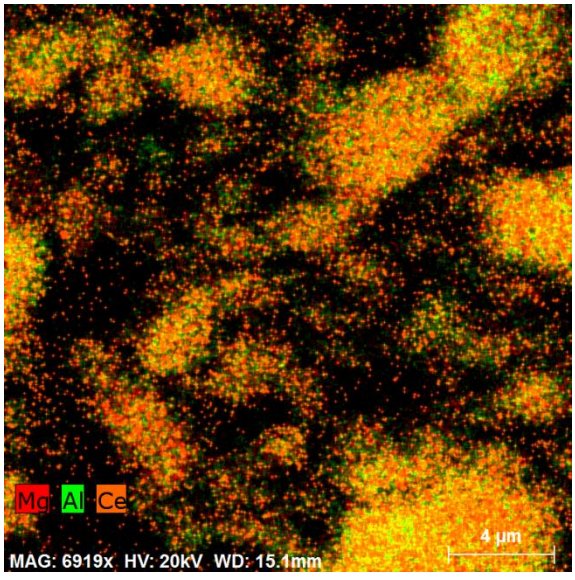


C

Figure S1. EDX maps of magnesium, aluminium and cerium atom distributions on the surface of Mg-Al-Ce oxide systems: A – Mg-Al-Ce-4, B – Mg-Al-Ce-2, C – Mg-Al-Ce-1.

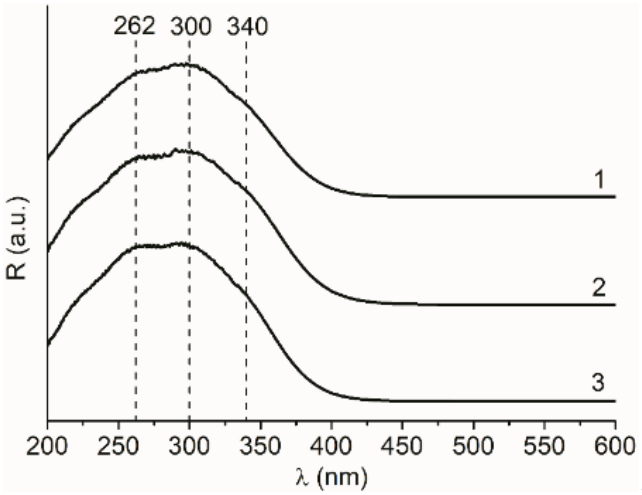


Figure S2. UV-vis DR spectra of samples after a treatment at 873 K:1 – Mg-Al-Ce-4, 2 – Mg-Al-Ce-2, 3 – Mg-Al-Ce-1.

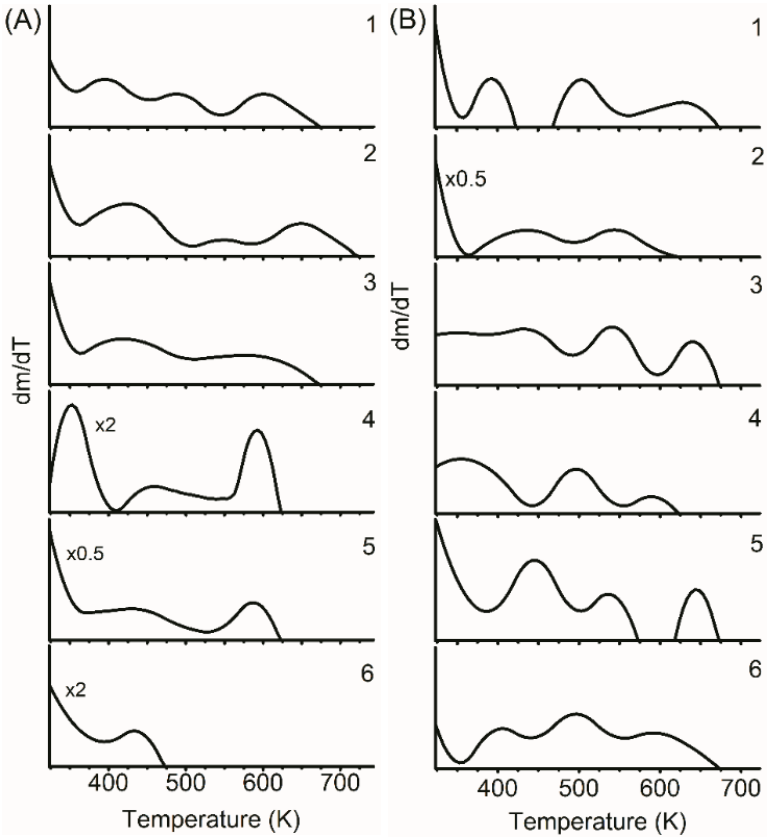


Figure S3. Differential QE-TD-curves of ammonia (A) and carbon dioxide (B) for the samples: 1 – Mg-Al-Ce-4, 2 – Mg-Al-Ce-2, 3 – Mg-Al-Ce-1, 4 – CeO_x, 5 – Al_2O_3, 6 – MgO.

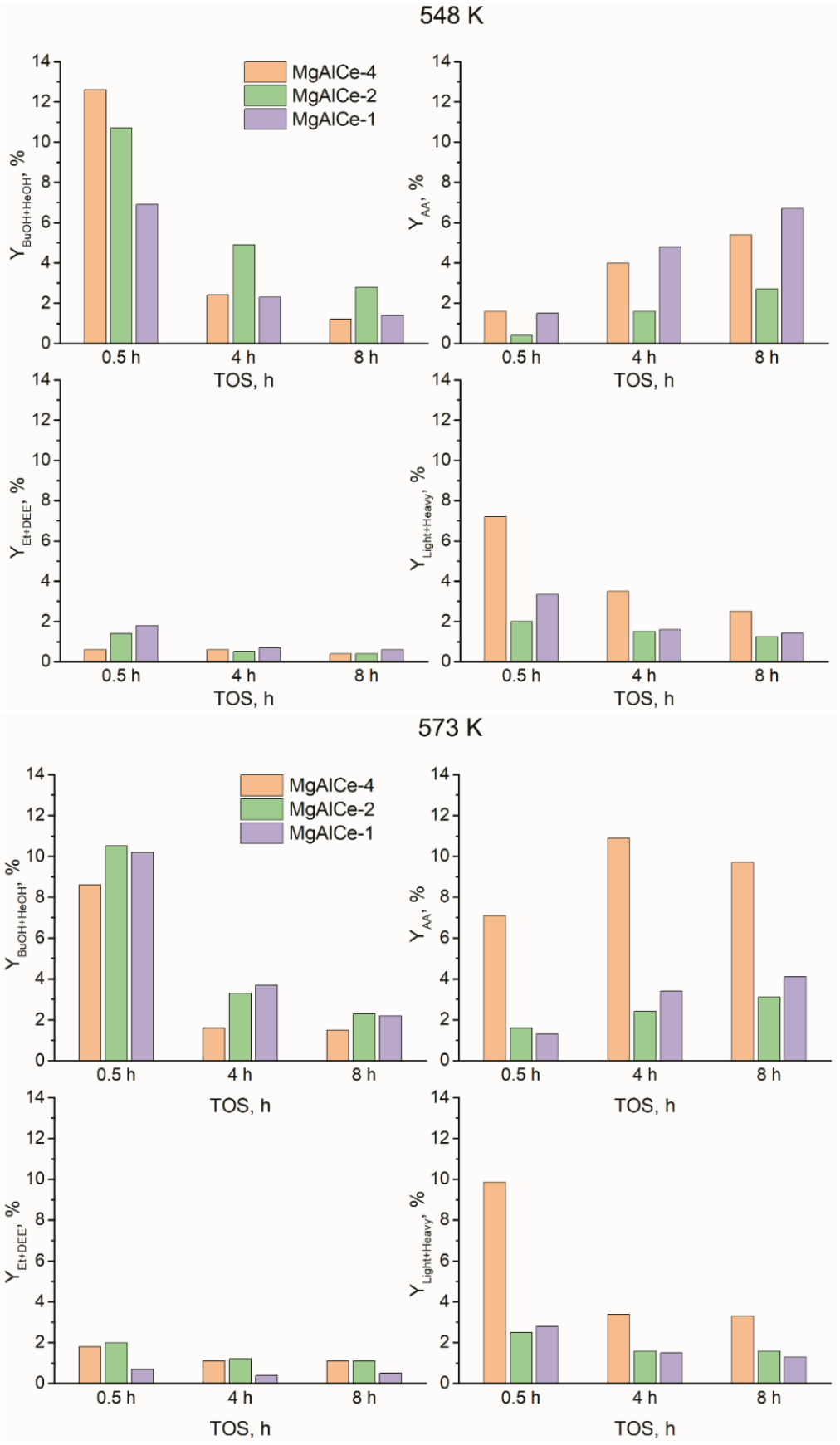


Figure S4. Yield of the main products in ethanol conversion over Mg-Al-Ce oxide catalysts in a flow reactor during different time on stream (548 and 573 K, atmospheric pressure, WHSV = 0.14 $g \cdot g_{cat}^{-1} \cdot h^{-1}$).

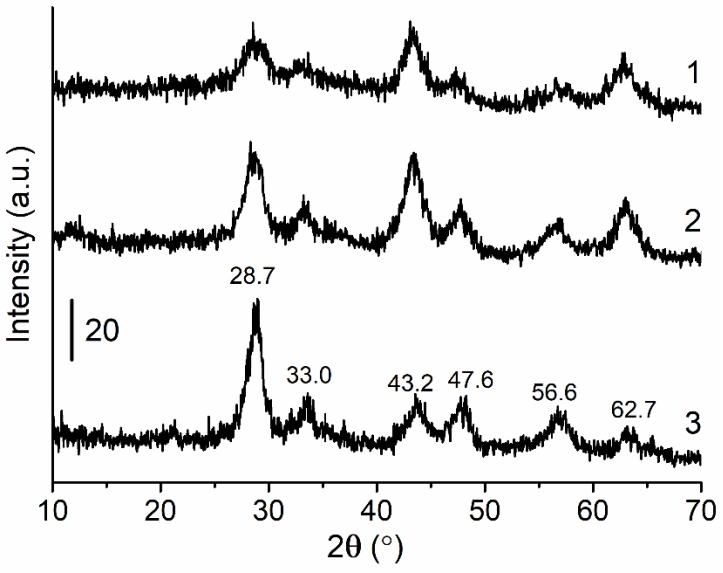
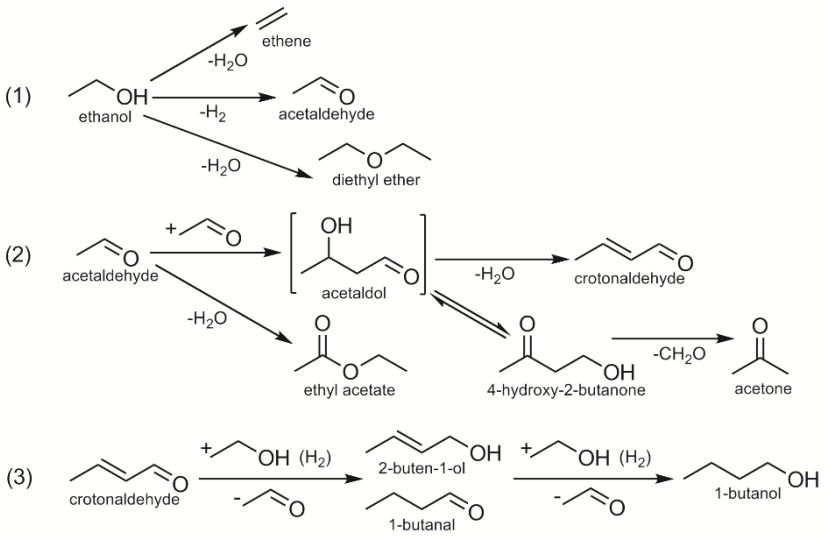
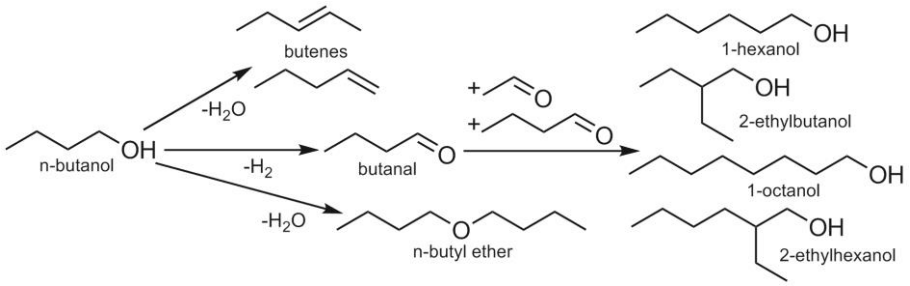


Figure S5. XRD patterns of the samples after 8 h time on stream of Guerbet coupling reaction of ethanol in their presence (T=573 K, atmospheric pressure, WHSV=0.14 $g \cdot g_{cat}^{-1} \cdot h^{-1}$) without subsequent calcination of the sample: 1– Mg-Al-Ce-4, 2– Mg-Al-Ce-2, 3– Mg-Al-Ce-1.



Scheme S1. The scheme of Guerbet condensation mechanism of ethanol into 1-butanol and side product formation over Mg-Al-Ce oxide catalysts.

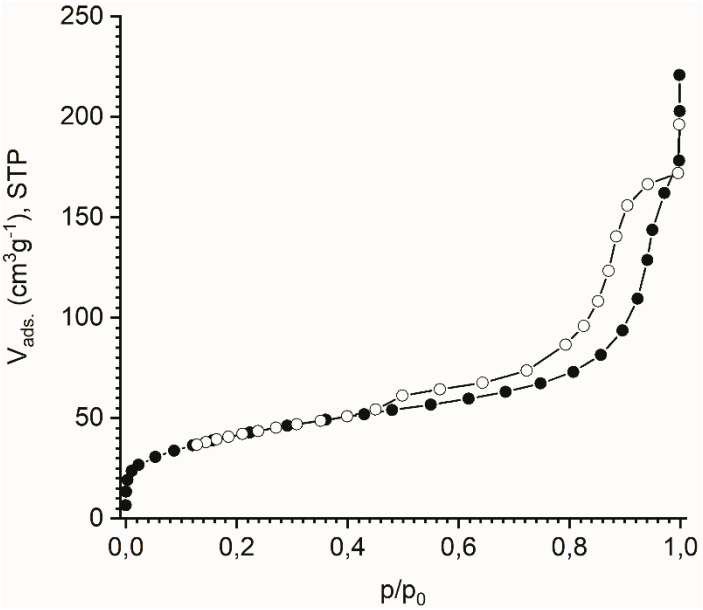


Scheme S2. The possible way to obtain higher alcohols from 1-butanol by Guerbet condensation.

Table S1. Textural characteristics (nitrogen ad(de)sorption, 77 K)[1] of Mg-Al-Ce-2 sample.

Sample	V_{Σ}[2], cm^3/g	V_{meso}[3], cm^3/g	$D_{meso,\ max}$[3], nm	V_{micro}[4], cm^3/g
Mg-Al-Ce-2	0.27	0.23	17	0.04

[1] Nitrogen adsorption-desorption isotherms for the Mg-Al-Ce-2 sample are shown below.



[2] total pore volume at $p/p_0 = 1.0$;

[3] calculations using the Barrett-Joyner-Halenda method;

[4] calculations using *t-plot* method.

Table S2. Indices of Guerbet coupling reaction of ethanol over Mg-Al-Ce oxide catalysts[a]

T, K	TOS, h	X_{EtOH}, %	S[b], %							Y_{BuOH}, %
			BuOH	HeOH	AA	Et	DEE	Light[c]	Heavy[d]	
Mg-Al-Ce-4										
548	0.5	22.0	50.3	6.8	7.5	0.5	2.1	17.8	15.0	11.0
	4	10.5	21.9	0.9	38.3	1.2	4.2	20.6	12.9	2.3
	8	9.5	13.1	0.0	56.5	0.7	3.4	19.9	6.4	1.2
573	0.5	27.4	29.3	2.3	26.0	1.0	5.4	27.6	8.4	8.0
	4	17.1	9.1	0.5	64.1	0.9	5.6	17.7	2.1	1.6
	8	15.6	9.1	0.3	62.2	1.3	5.7	19.2	2.3	1.4
Mg-Al-Ce-2										
548	0.5	14.5	68.1	5.7	3.0	2.2	7.2	3.5	10.3	9.8
	4	8.6	53.7	3.8	19.0	1.3	4.4	6.1	11.6	4.6
	8	7.2	37.2	1.8	38.2	1.1	4.1	6.9	10.7	2.7
573	0.5	16.7	58.7	4.5	9.4	3.3	8.8	9.9	5.4	9.8
	4	8.4	37.6	1.6	28.3	3.3	10.5	8.9	9.9	3.2
	8	8.1	27.8	1.1	38.3	3.6	10.0	10.0	9.2	2.2
Mg-Al-Ce-1										
548	0.5	13.6	47.1	3.9	11.2	4.5	8.7	11.7	13.0	6.4
	4	9.4	22.6	1.5	51.2	2.0	5.8	12.0	4.9	2.5
	8	10.1	12.6	1.2	66.2	1.7	4.1	10,7	3.6	1.4
573	0.5	15.0	62.9	5.0	8.9	1.3	3.2	10.6	8.0	9.4
	4	8.9	38.9	2.5	37.8	1.0	2.9	8.7	8.1	3.5
	8	8.1	25.4	1.5	50.5	1.0	4.8	6.5	10.3	2.1

[a] WHSV = 0.14 $g \cdot g_{cat}^{-1} \cdot h^{-1}$, atmospheric pressure.

[b] The selectivities reported in the table are normalized per amount of C moles.

[c] Light – sum of acetone, ethyl acetate, 1-butene, 1-butanal, 1,3-butadiene and other light fractions.

[d] Heavy – sum of other products of condensations: alcohols (2-ethyl-1-butanol, 2-ethyl-1-hexanol and 1-octanol), aldehydes, ketones, aromatics.