Electronic Supplementary Material

Investigation of the effect of thermal annealing of Ni-Cobaltite nanoparticles on their structure, electronic properties and performance as catalysts for the total oxidation of di(methyl)ether (DME).

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Section 1 : XPS details: Results of curve-fitting on the Co 2p, Ni 2p and O1s binding energies and relative atomic percentage for the five sets of catalysts.

Table ESM1: Results of curve-fitting on the Co 2p binding energies and relative atomic percentage for the five sets of catalysts.

Catalysts	Parameters	Co 2p3/2			Co 2p1/2		
	Species	Co^{2+}	Co^{3+}	**Co^{3+}/Co^{2+}**	Co^{2+}	Co^{3+}	**Co^{3+}/Co^{2+}**
Co_3O_4	BE (eV)	779.35	780.86	4.32	795.18	797.14	4.12
	RA (%)	18.81	81.19		19.54	80.46	
	Species	Co^{2+}	Co^{3+}	**Co^{3+}/Co^{2+}**	Co^{2+}	Co^{3+}	**Co^{3+}/Co^{2+}**
$(NiCo_2O_4)_{500}$	BE (eV)	779.41	781.57	3.50	795.47	796.98	3.26
	RA (%)	22.20	77.80		23.47	76.53	
	Species	Co^{2+}	Co^{3+}	**Co^{3+}/Co^{2+}**	Co^{2+}	Co^{3+}	**Co^{3+}/Co^{2+}**
$(NiCo_2O_4)_{450}$	BE (eV)	779.27	780.98	2.91	795.66	797.41	2.68
	RA (%)	25.57	74.43		27.18	72.82	
	Species	Co^{2+}	Co^{3+}	**Co^{3+}/Co^{2+}**	Co^{2+}	Co^{3+}	**Co^{3+}/Co^{2+}**
$(NiCo_2O_4)_{350}$	BE (eV)	779.93	781.58	1.92	795.36	796.84	2.03
	RA (%)	34.30	65.70		33.03	66.97	
Ni_2O_3	-	-	-	-	-	-	-

Note: BE refers to binding energy, and RA refers to the relative area of the peak.

Table ESM2: Results of curve-fitting on the Ni 2p binding energies and relative atomic percentage for the five sets of catalysts.

Catalysts	Parameters	Ni 2p3/2			Ni 2p1/2		
Co_3O_4	-	-	-	**-**	-	-	**-**
	Species	Ni^{2+}	Ni^{3+}	**Ni^{3+}/Ni^{2+}**	Ni^{2+}	Ni^{3+}	**Ni^{3+}/Ni^{2+}**
$(NiCo_2O_4)_{500}$	BE (eV)	854.20	855.84	3.13	871.57	873.20	3.67
	RA (%)	24.20	75.80		21.42	78.58	
	Species	Ni^{2+}	Ni^{3+}	**Ni^{3+}/Ni^{2+}**	Ni^{2+}	Ni^{3+}	**Ni^{3+}/Ni^{2+}**
$(NiCo_2O_4)_{450}$	BE (eV)	854.19	855.95	2.63	871.41	872.74	2.61
	RA (%)	27.57	72.43		27.70	72.30	
	Species	Ni^{2+}	Ni^{3+}	**Ni^{3+}/Ni^{2+}**	Ni^{2+}	Ni^{3+}	**Ni^{3+}/Ni^{2+}**
$(NiCo_2O_4)_{350}$	BE (eV)	854.18	855.85	2.06	871.37	872.76	2.23
	RA (%)	32.72	67.28		30.98	69.02	
	Species	Ni^{2+}	Ni^{3+}	**Ni^{3+}/Ni^{2+}**	Ni^{2+}	Ni^{3+}	**Ni^{3+}/Ni^{2+}**
Ni_2O_3	BE (eV)	854.42	856.27	1.19	871.65	873.25	1.07
	RA (%)	45.60	54.40		48.36	51.64	

Note: BE refers to binding energy, and RA refers to the relative area of the peak.

Table ESM3: Results of curve-fittings on the O1s binding energies and relative atomic percentage for the four sets of catalysts

Catalysts	Parameters	O 1s			
	Species	O^{2-}	CO_3^{2-}	OH^-	O_{Lat}/O_{Ads}
$(NiCo_2O_4)_{500}$	BE (eV)	530.47	531.88	532.96	1.68
	RA (%)	62.71	29.20	8.09	
	Species	O^{2-}	CO_3^{2-}	OH^-	O_{Lat}/O_{Ads}
$(NiCo_2O_4)_{450}$	BE (eV)	530.52	531.75	532.70	1.47
	RA (%)	59.44	28.03	12.53	
	Species	O^{2-}	CO_3^{2-}	OH^-	O_{Lat}/O_{Ads}
$(NiCo_2O_4)_{350}$	BE (eV)	529.74	531.03	532.09	1.32
	RA (%)	56.95	27.12	15.93	
	Species	O^{2-}	CO_3^{2-}	OH^-	O_{Lat}/O_{Ads}
Co_3O_4	BE (eV)	529.91	531.04	532.02	1.18
	RA (%)	54.14	15.41	30.45	
	Species	O^{2-}	CO_3^{2-}	OH^-	O_{Lat}/O_{Ads}
Ni_2O_3	BE (eV)	530.03	531.16	532.13	1.11
	RA (%)	52.71	12.85	34.44	

Note: BE refers to the binding energy; O_{Lat} refers to the lattice oxygen; O_{Ads} refers to the adsorption oxygen; RA refers to the relative area of the peak.

Section 2: Catalytic performance comparison with the literature data.

Table ESM4. Comparison of the $[NiCo_2O_4]_{500}$ catalytic efficiency (T_{50}, T_{90}) to that of the single and mixed oxides reported catalysts from the literature.

Material	Weight (mg)	Gas composition	T_{50} (°C)	T_{90} (°C)	Refs.
Singles oxides					
Co_3O_4	60	5% DME/20% O_2 in Ar	300	325	TW
Fe_3O_4	100	900 ppm DME /20% O_2 in He	310	345	[1]
CuO	100	900 ppm DME /20% O_2 in He	311	358	
α-MnO_2	100	2% DME /20% O_2 in He	205	238	[2]
Mixed oxides					
$[NiCo_2O_4]_{500}$	60	5% DME/20% O_2 in Ar	200	240	TW
$Fe_{0,67}Cu_{0,33}$	100	900 ppm DME /20% O_2 in He	265	292	
$Fe_{0,50}Cu_{0,50}$	100	900 ppm DME /20% O_2 in He	278	313	[1]
$Fe_{0,33}Cu_{0,67}$	100	900 ppm DME /20% O_2 in He	287	321	
$Co_{2.1}Fe_{0.9}O_4$	20	1% DME/10% O_2 in Ar	356	409	[3]

***Note**: TW stand for this work, T_{50} and T_{90} stand for temperature at 50 and 90% conversion of DME.*

References

1. Smyrnioti M., Ioannides T. Dimethyl Ether Oxidation over Copper Ferrite Catalysts . *Catalysts 2022, 12, 604*.

2. Cheng, G.; Yu, L.; He, B.; Sun, M.; Zhang, B.; Ye, W.; Lan, B. Catalytic Combustion of Dimethyl Ether over a-MnO_2 Nanostructures with Different Morphologies. *Appl. Surf. Sci.* 2017, *409*, 223–231.

3. Tian, Z.-Y.; Kouotou, P.M.; El Kasmi, A.; Tchoua Ngamou, P.H.; Kohse-Hoïnghaus, K.; Vieker, H.; Beyer, A.; Gölzhäuser, A. Low-Temperature Deep Oxidation of Olefins and DME over Cobalt Ferrite. Proc. Combust. Inst. 2015, 35, 2207–2214.