catalysts

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Supplementary Material

Green epoxidation of olefins with Zn_xAl/Mg_xAl-LDH compounds: influence of the chemical composition

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Table S1. Structural parameters of freshly prepared samples.

HT Samples	*a* (Å)	*c* (Å)	D_{003} (nm) *	D_{110} (nm) *	I_{003}/I_{110}	Impurities
Zn_2Al	3.055	22.156	25.1	35.6	7.1	
$Zn_{2.5}Al$	3.059	22.295	19.0	26.9	7.7	small amorphous peak
Zn_3Al	3.066	22.476	21.8	30.2	7.1	
Zn_4Al	3.066	22.486	23.3	32.0	8.6	$Zn_3(OH)_4(NO_3)_2$
Zn_5Al	3.068	22.547	21.8	29.2	6.0	$Zn_3(OH)_4(NO_3)_2$
Zn_2Al	3.055	22.270	23.4	22.8	7.6	amorphous peak
$Zn_{2.5}Al$	3.062	22.377	18.3	28.8	6.3	small amorphous peak
Zn_3Al	3.065	22.420	17.7	31.4	6.2	$Zn_3(OH)_4(NO_3)_2$
Zn_4Al	3.070	22.624	16.2	27.3	5.9	$Zn_3(OH)_4(NO_3)_2$
Zn_5Al	3.067	22.507	23.1	31.0	7.8	$Zn_3(OH)_4(NO_3)_2$
Zn_3MgAl	3.065	22.656	12.3	20.3	4.8	
Zn_2Mg_2Al	3.065	22.680	5.5	10.7	3.4	amorphous
$ZnMg_3Al$	3.064	22.629	5.0	9.7	2.9	
Mg_2Al	3.049	23.063	9.2	22.1	4.0	
$Mg_{2.5}Al$	3.054	23.307	8.1	12.9	4.9	
Mg_3Al	3.066	23.592	8.2	24.2	3.7	
Mg_4Al	3.061	23.272	7.6	13.4	3.7	
Mg_5Al	3.060	24.064	4.2	6.9	2.7	

* Crystallite dimensions (with Debye-Scherrer equation) and obtained from FWHM of 003 and 110 reflections for HT and RHT samples

Table S2. Structural parameters of calcined samples.

CHT Samples	ZnO-zincite Type Phase [Zn(Al)O]				MgO-Periclase Type Phase [Mg(Al)O]	
	a **(Å)**	***c*** **(Å)**	**Vol (Å^3)**	**D_{101} (nm)**	***a*** **(Å)**	**D_{200} (nm)**
Standard ZnO ICDD-36-1451	3.250	5.207	47.62	-	-	-
CHT-Zn_5Al	3.240	5.193	47.20	17.0	-	-
CHT-Zn_4Al	3.240	5.198	47.25	12.2	-	-
CHT-Zn_3Al	3.238	5.200	47.21	7.3	-	-
CHT-$Zn_{2.5}Al$	3.250	5.200	47.48	4.1	-	-
CHT-Zn_2Al	3.24	5.198	47.25	3.8	-	-
CHT-Zn_3MgAl	3.244	5.191	47.31	5.8	-	-
CHT-Zn_2Mg_2Al	3.240	5.190	47.24	3.7	4.182	2.3
CHT-$ZnMg_3Al$	3.240	5.170	46.85	2.7	4.194	2.7
Standard MgO ICDD 45-0946	-	-	-	-	4.211	-
CHT Mg_5Al	-	-	-	-	4.187	4.0
CHT Mg_4Al	-	-	-	-	4.176	3.4
CHT Mg_3Al	-	-	-	-	4.142	3.1
CHT $Mg_{2.5}Al$	-	-	-	-	4.133	6.0
CHT Mg_2Al	-	-	-	-	4.127	8.0

* Crystallite dimensions (with Debye-Scherrer equation) obtained from FWHM of 200 reflection for Mg(Al)O and 101 reflection for Zn(Al)O

Table S3. Structural parameters of reconstructed samples.

RHT Samples	HT phase					Oxide Phase Zn(Al)O			
	***a* (Å)**	***c* (Å)**	**D_{003} (nm)**	**D_{110} (nm)**	**I_{003}/I_{110}**	***a* (Å)**	***c* (Å)**	**Vol (Å^3)**	**D_{101} (nm)**
RHT-Zn_2Al	3.057	22.360	17.9	22.7	6.9	3.255	5.080	46.64	7.6
RHT-$Zn_{2.5}Al$	3.065	22.338	17.9	24.3	5.3	3.252	5.280	48.37	17.2
RHT-Zn_3Al	3.051	22.546	8.8	16.5	4.7	3.269	5.240	47.62	15.9
RH-Zn_4Al	3.062	22.504	16.5	26.9	5.1	3.246	5.195	47.40	20.2
RHT-Zn_5Al	3.059	22.375	19.4	34.6	4.6	3.241	5.198	47.29	24.4
RHT-Zn_3MgAl	3.052	22.547	21.4	18.8	6.4	3.250	5.220	47.72	14.3
RHT-Zn_2Mg_2Al	3.044	22.637	9.0	14.0	4.3	3.245	5.191	47.34	18.1
RHT-$ZnMg_3Al$	3.060	23.051	10.1	17.4	3.1	3.246	5.197	47.43	15.7
RHT-Mg_4Al	3.073	23.164	8.2	9.6	3.5	-	-	-	-
RHT-Mg_2Al	3.058	23.288	9.9	11.6	6.7	-	-	-	-
RHT-$Mg_{2.5}Al$	3.062	23.318	11.5	18.0	7.2	-	-	-	-
RHT-Mg_3Al	3.063	23.363	12.7	21.1	6.8	-	-	-	-
RH-Mg_4Al	3.073	23.164	8.2	9.6	3.5	-	-	-	-
RHT-Mg_5Al	3.074	23.773	6.3	13.8	3.7	-	-	-	-

* Crystallite dimensions (with Debye-Scherrer equation) and obtained from FWHM of 003 and 110 reflections for HT and RHT samples and 101 reflection for Zn(Al)O