Electronic Supporting Information

Magnesium-modified Co_3O_4 catalyst with remarkable performance for toluene low temperature deep oxidation

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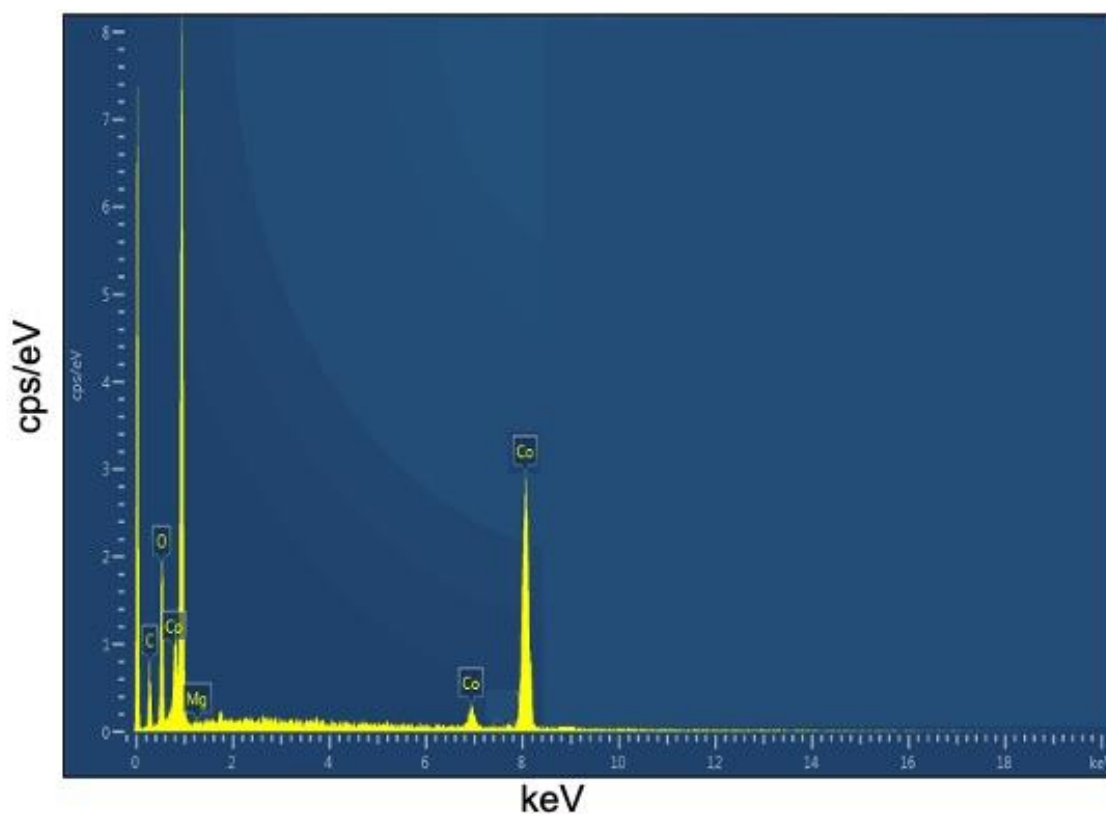# Section S1: Chemical composition analysis by EDS

Figure S1: EDS pattern of $MgCo_2O_4$ prepared by coprecipitation technique.

Table S1: EDS bulk elemental analysis of $MgCo_2O_4$

Elements	Apparent concentration	k Ratio	wt%	wt% Sigma	Atomic percentage
C	1.80	0.01799	7.73	2.50	10.47
O	22.25	0.07487	45.02	2.07	47.59
Mg	0.08	0.00050	15..41	0.60	13.33
Co	9.56	0.09561	31.84	1.67	28.61
Total:			100.00		100.00

Section S2: Computational Details

Spin polarized Born-Oppenheimer molecular dynamics (MD) simulations were performed for a total time of 10 ps with a time step of 0.5 fs at the Γ point using the CP2K/Quickstep package.1 The NVT ensemble was employed with a Nosé-Hoover thermostat [76,77] with target temperatures of 550 K and a time constant of 1 ps. The PBE-D3 functional with Hubbard [78] correction terms of U =2.0 eV [60] for Co was used to treat exchange and correlation. The Goedecker-Teter-Hutter (GTH) pseudopotentials [79] were used to treat the core electrons. The basis sets consist of plane waves with a cut-off of 500 Ry together with double-ζ quality local basis functions containing a single set of polarization functions (DZVP). The (111) surface can exhibit five different terminations, we used the termination with the smallest number of dangling bonds. This termination ends with metal ions, that are tetrahedrally or octahedrally coordinated with one or two dangling bonds, while one quarter of the oxygen atoms have one dangling bond. The Co_3O_4 and $MgCo_2O_4$ interface was modelled by stoichiometric slabs consisting of 13 atomic layers and two toluene molecules. The bottom 6 layers of the slab were kept frozen at their bulk positions, and the remaining atoms were fully relaxed and mobile as was the toluene molecules in the orthorhombic supercell with (2x2) periodicity in the lateral directions (x, y) and dimensions 19.8127 Å × 11.4389 Å × 40.0 Å ($MgCo_2O_4$: 20.0234 Å × 11.5605 Å × 40.0 Å).

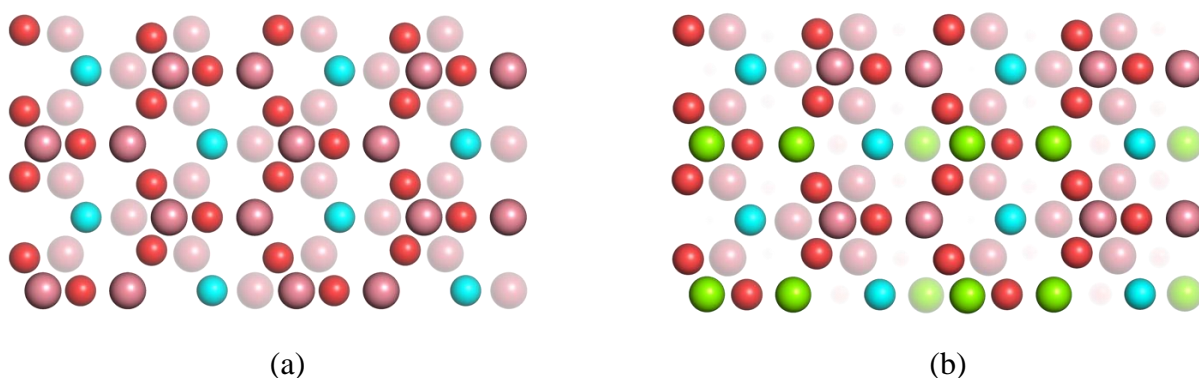| (a) | (b) |

Figure S2: Top views of: (a) Co_3O_4(111) and (b) $MgCo_2O_4$(111) surfaces. Mg: green, Co: pink, slab oxygens: red, unsaturated slab oxygen with only 3 metal ions neighbors: cyan.

Section S3: Comparison of the catalytic $MgCo_2O_4$ performance towards toluene oxidation with results in literature.

Table S2: Catalytic performance and test conditions of toluene over $MgCo_2O_4$, Co_3O_4 and other related catalysts earlier reported in the literature.

Catalysts	Masse (g)	Concentration (ppm)	WHSV (mL $g_{cat}^{-1}h^{-1}$)	$T_{90\%}$	$T_{100\%}$	Reference
Co_3O_4	0.06	500	20 000		315	This work
Co_3O_4 microspheres		1000	20 000	285		[58]
Co_3O_4 NS		1000	20 000	-	300	[65]
$Cu-Co_3O_4$		1000	20000	219	240	[66]
Co_3O_4	0.2	1000	20000	316	340	[44]
$MgCo_2O_4$	0.06	500	20 000	250	255	This work
$6.4Au/bulkCo_3O_4$		1000	20 000	277	-	[52]
$7.4 Au/Co_3O_4$		1000	20 000	250		[58]
MnAl/Na-L(II)	0.5	500	10000	260	-	[76]
Pd/Co_3AlO	0.6	1000	30 000	230	290	[67]