

Supporting Information

Perovskite-type LaCoO_3 as an Efficient and Green Catalyst for Sustainable Partial Oxidation of Cyclohexane

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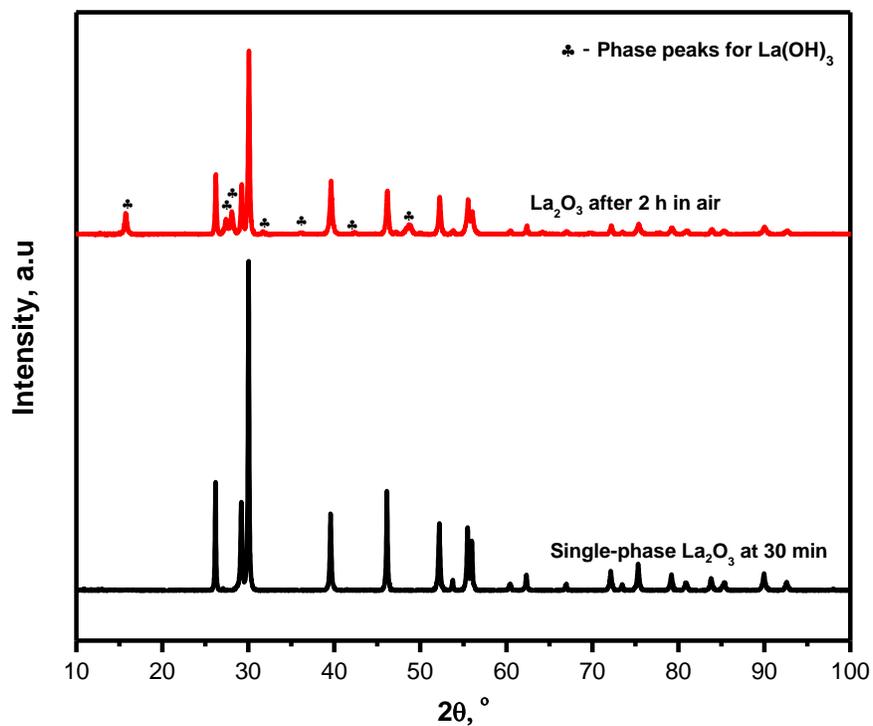


Figure S1. XRD patterns for La_2O_3 analyzed within half an hour and 2 hours after removal from furnace.

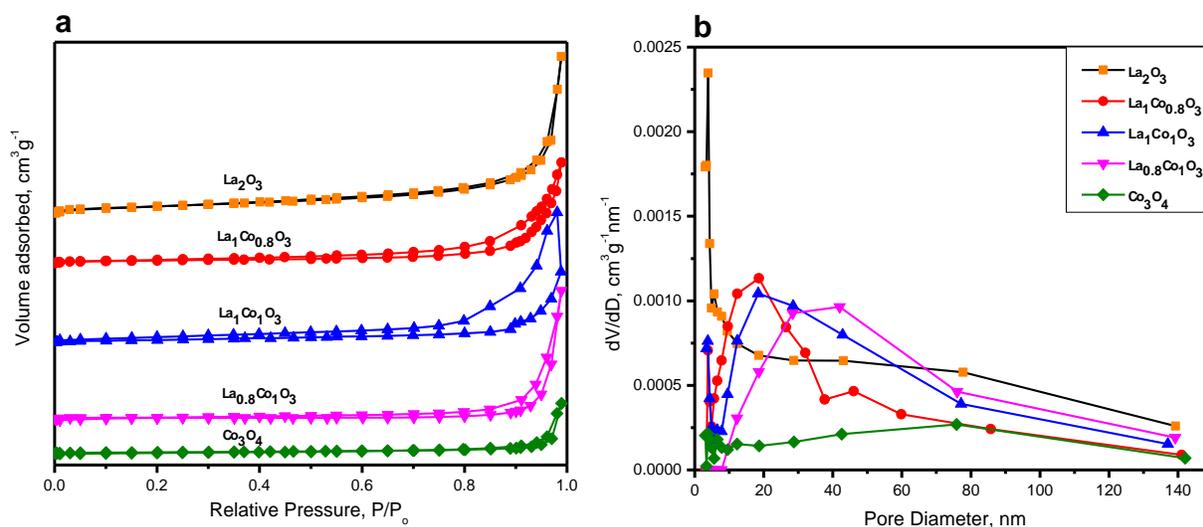


Figure S2. The N_2 adsorption-desorption isotherms (a) and their corresponding BJH pore size distribution (b) of La_2O_3 , $\text{La}_1\text{Co}_{0.8}\text{O}_3$, $\text{La}_1\text{Co}_1\text{O}_3$, $\text{La}_{0.8}\text{Co}_1\text{O}_3$ and Co_3O_4 .

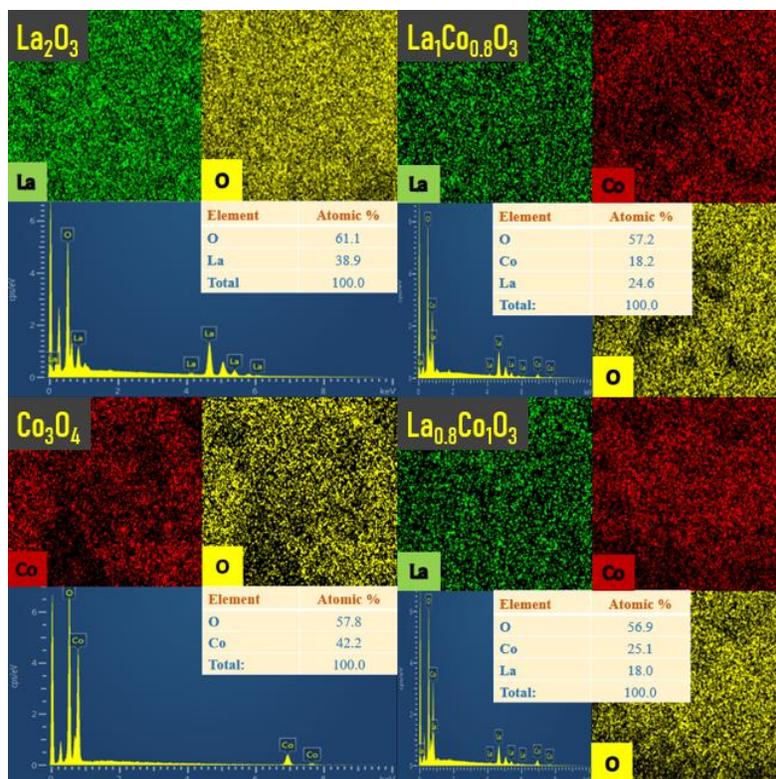


Figure S3. The EDX mappings for La_2O_3 , $\text{La}_1\text{Co}_{0.8}\text{O}_3$, $\text{La}_{0.8}\text{Co}_1\text{O}_3$ and Co_3O_4 .

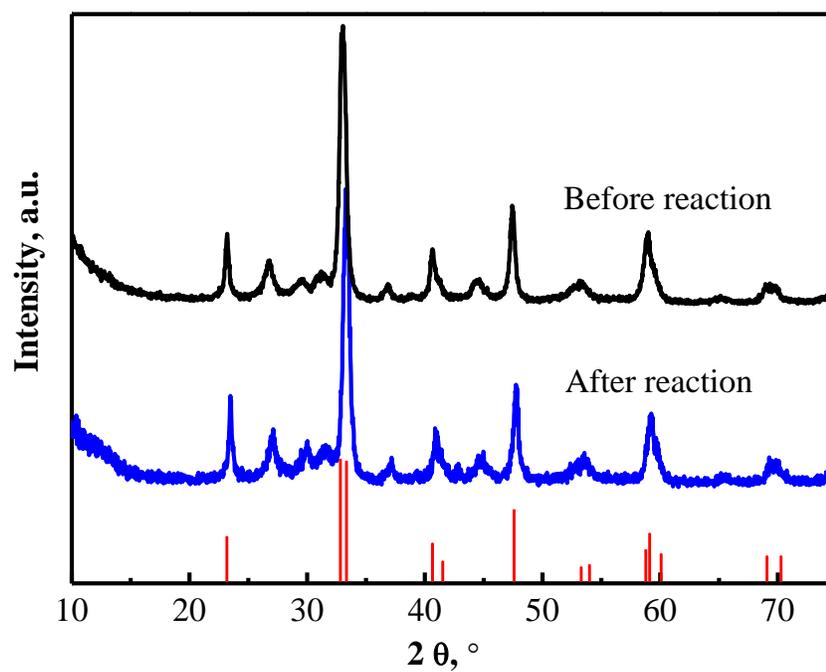


Figure S4. XRD patterns of catalyst $\text{La}_1\text{Co}_1\text{O}_3$ before and after reaction.

Table S1. Structural Parameters of La₂O₃, La₁Co_{0.8}O₃, La₁CoO₃, La_{0.8}CoO₃ and Co₃O₄ from Rietveld Refinement.

	La ₂ O ₃	La ₁ Co _{0.8} O ₃	La ₁ CoO ₃	La _{0.8} CoO ₃	Co ₃ O ₄
Phase 1 (LaCoO ₃)					
a / Å		5.443	5.443	5.442	
c / Å		13.109	13.109	13.103	
Vol / Å ³		336.316	336.305	336.011	
Space group		<i>R3̄c</i>	<i>R3̄c</i>	<i>R3̄c</i>	
Phase %		77.11	100	79.91	
Phase 2 (La ₂ O ₃)					
a / Å	3.938	3.933			
c / Å	6.128	6.140			
Vol / Å ³	82.279	82.432			
Space group	<i>P6₃/mmc</i>	<i>P6₃/mmc</i>			
Phase %	100	22.85			
Phase 3 (Co ₃ O ₄)					
a / Å				8.071	8.065
Vol / Å ³				525.699	524.572
Space group				<i>Fd3̄m</i>	<i>Fd3̄m</i>
Phase %				20.09	100
G.O.F	1.12	1.15	1.12	1.03	1.07
R _p	5.14	6.63	7.12	5.96	5.63
R _{wp}	8.99	9.37	9.18	8.86	7.37
R _{exp}	8.01	8.11	10.29	8.64	6.88

Table S2. Refined Unit Cell Lattice Parameters of La₁CoO₃.

Site	x	y	z	Occ	Beq	Co-O, Å	Co-O-Co, °
La	0	0	0.25	1	1	1.931	165
Co	0	0	0	1	1		
O	0.443	0	0.25	1	1		

Table S3. Surface Atomic Concentrations of La₂O₃, La₁Co_{0.8}O₃, La₁CoO₃, La_{0.8}CoO₃ and Co₃O₄ Measured by XPS.

Catalyst	La (%)	Co (%)	O (%)
La ₂ O ₃	26.35	-	73.65
La ₁ Co _{0.8} O ₃	21.77	7.73	70.5
LaCoO ₃	19.31	10.81	69.88
La _{0.8} CoO ₃	16.71	14.08	69.21
Co ₃ O ₄	-	31.7	68.3