

Supporting Information

Selective Cyclohexene Oxidation with O₂, H₂O₂ and *tert*-Butyl Hydroperoxide over Spray-Flame Synthesized LaCo_{1-x}Fe_xO₃ Nanoparticles

Julia Büker,^[a] Baris Alkan,^[b] Qi Fu,^[a] Wei Xia,^[a] Jonas Schulwitz,^[a] Daniel Waffel,^[a] Tobias Falk,^[a] Christof Schulz,^[b] Hartmut Wiggers,^[b] Martin Muhler,^{[a],[c]} and Baoxiang Peng*^{[a],[c]}

^a Laboratory of Industrial Chemistry, Ruhr-University Bochum, 44780 Bochum, Germany

^b IVG, Institute for Combustion and Gas Dynamics – Reactive Fluids and CENIDE, Center for Nanointegration Duisburg-Essen, University of Duisburg-Essen, 47057 Duisburg, Germany

^c Max Planck Institute for Chemical Energy Conversion, 45470 Mülheim an der Ruhr, Germany

*Corresponding author. Email: baoxiang.peng@techem.rub.de

Table S1. Bulk chemical composition of $\text{LaCo}_{1-x}\text{Fe}_x\text{O}_3$ catalysts calculated by EDX measurements at STEM mode.

Catalysts	La/(Co+Fe)	Fe/(Fe+Co)
LaCoO_3	1.10 ± 0.03	-
$\text{LaCo}_{0.8}\text{Fe}_{0.2}\text{O}_3$	1.19 ± 0.16	0.20 ± 0.03
$\text{LaCo}_{0.7}\text{Fe}_{0.3}\text{O}_3$	1.10 ± 0.12	0.29 ± 0.01
$\text{LaCo}_{0.6}\text{Fe}_{0.4}\text{O}_3$	1.14 ± 0.04	0.36 ± 0.01

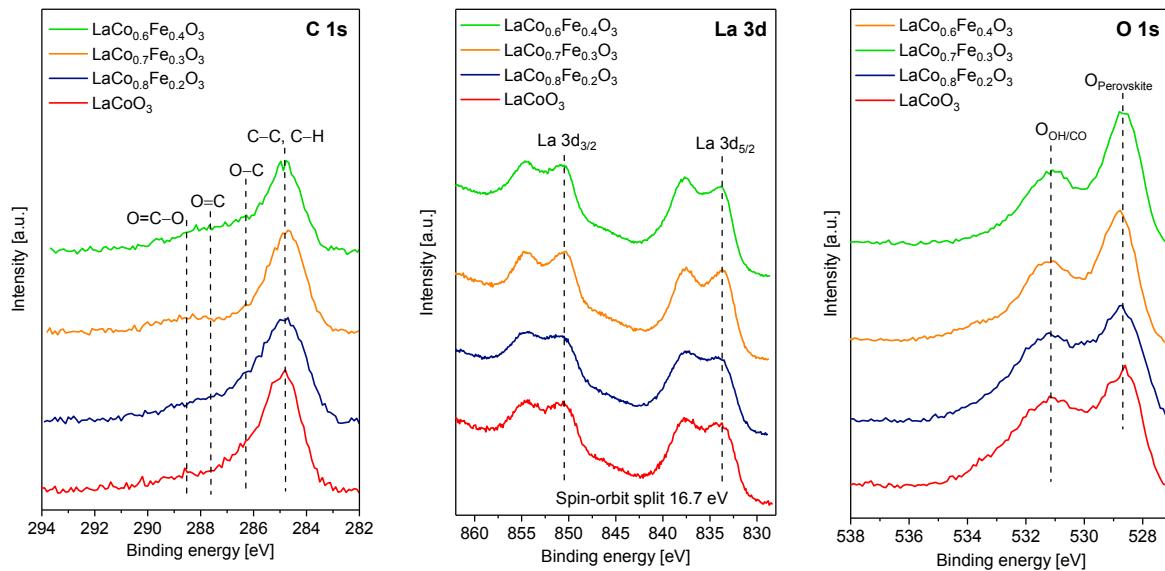


Figure S1. XP spectra of the C 1s, La 3d and O 1s regions of the $\text{LaCo}_{1-x}\text{Fe}_x\text{O}_3$ samples.

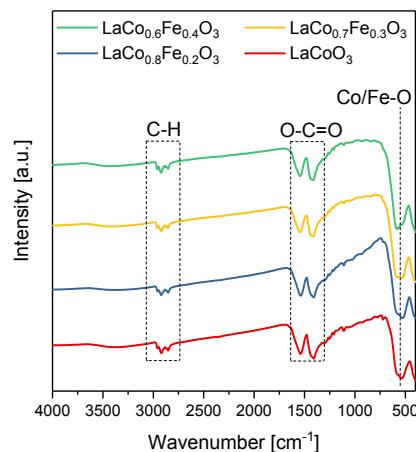


Figure S2. FT-IR spectra of the $\text{LaCo}_{1-x}\text{Fe}_x\text{O}_3$ samples.

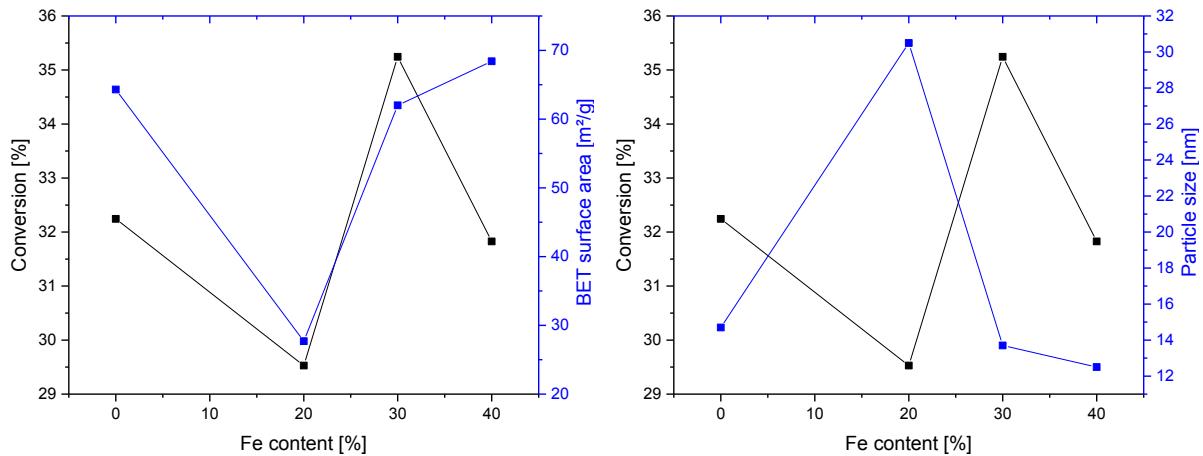


Figure S3. Correlations of cyclohexene conversion with BET surface areas (left) and particle sizes (right) after 2 h reaction over different $\text{LaCo}_{1-x}\text{Fe}_x\text{O}_3$ catalysts.

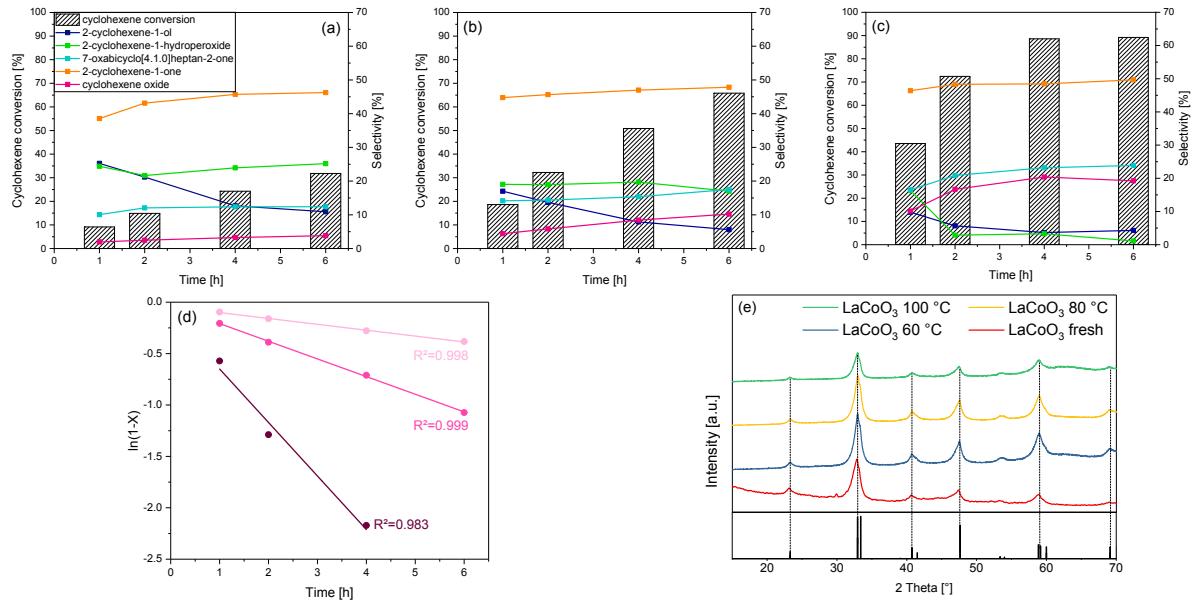


Figure S4. Effect of temperature on cyclohexene oxidation over LaCoO_3 at 60 (a), 80 (b) and 100 °C (c), linearized plot of the conversion as a function of time (d) and XRD patterns of used catalysts (e) (red: cyclohexene conversion, dark blue: 2-cyclohexene-1-ol, orange: 2-cyclohexene-1-one, green: 2-cyclohexene-1-hydroperoxide, pink: cyclohexene oxide, light blue: 7-oxabicyclo[4.1.0]heptan-2-one).

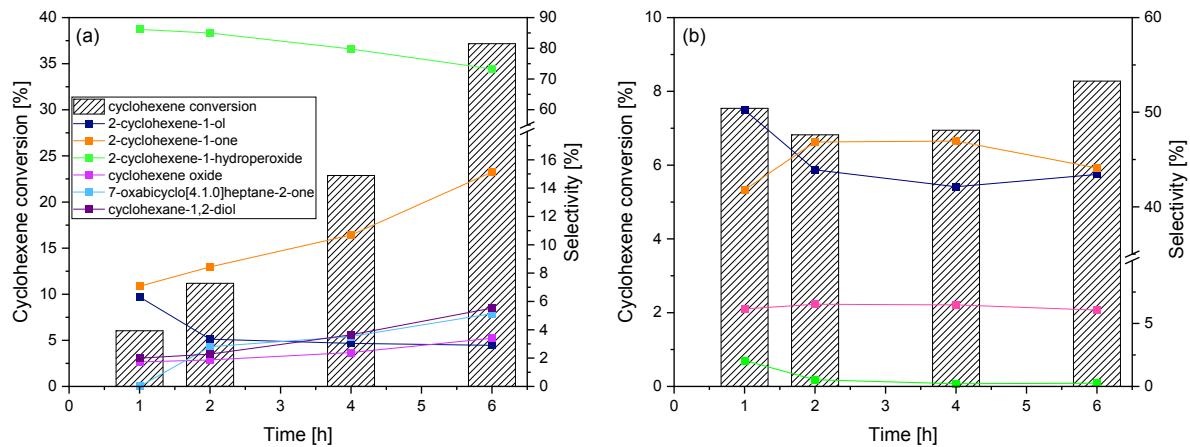


Figure S5. Cyclohexene oxidation under standard conditions in the absence of a catalyst (a) and in the presence of LaCoO_3 in N_2 atmosphere.

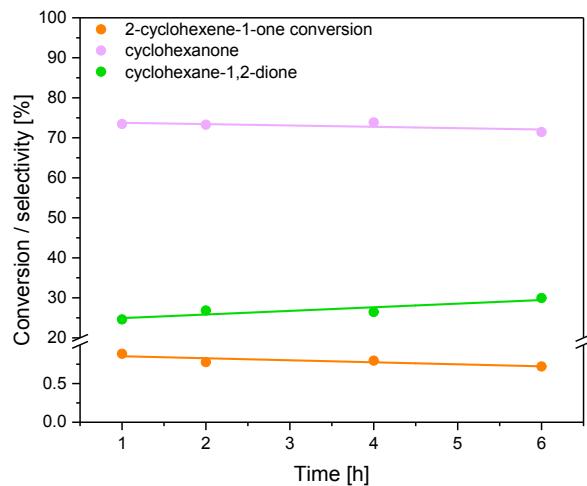


Figure S6. Oxidation of 2-cyclohexene-1-one with O_2 over LaCoO_3 under standard conditions.

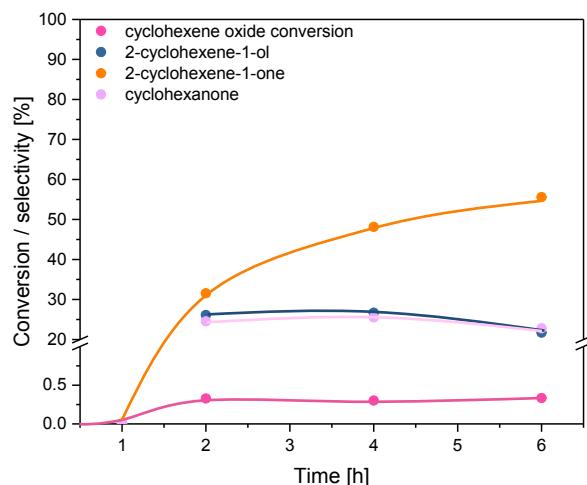
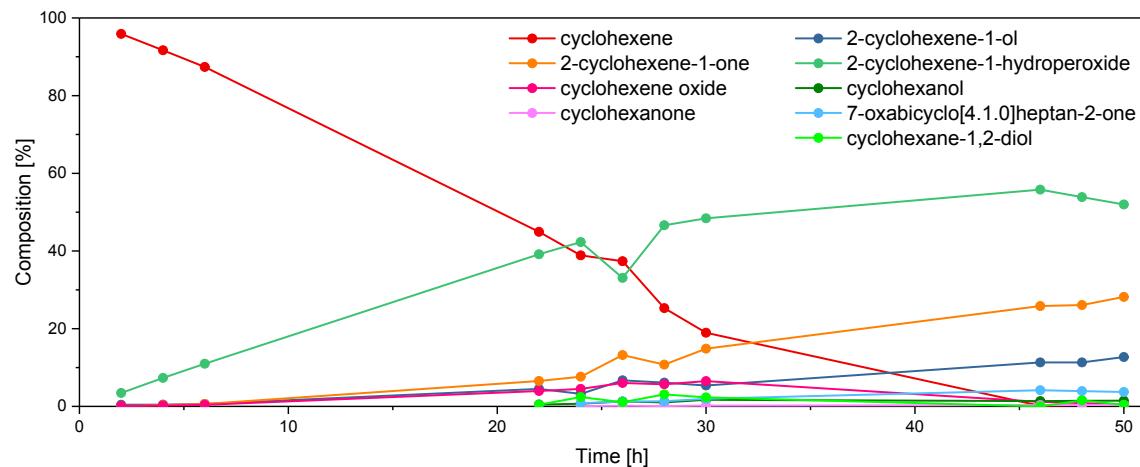


Figure S7. Oxidation of cyclohexene oxide with O_2 over LaCoO_3 under standard conditions.



).

Figure S8. Synthesis of 2-cyclohexene-1-hydroperoxide.

Table S2. Decomposition of 2-cyclohexene-1-hydroperoxide over LaCoO₃.

Time [h]	Composition [%]						
							others ^[a]
0	0.0	16.1	30.0	45.9	0.9	4.1	3.1
1	0.0	16.0	32.6	41.9	0.8	4.4	4.2
2	0.0	16.8	35.0	38.3	0.8	4.8	4.4
4	0.0	18.1	39.5	31.4	0.8	5.5	4.7
6	0.0	18.9	43.4	26.0	0.8	6.0	5.0
Δ	0.0	+ 2.8	+ 13.4	- 19.9	- 0.1	+ 1.9	+ 1.9

^[a] Others are cyclohexanone, cyclohexanol and cyclohexane-1,2-diol