

Thermocatalytic Performance of $\text{LaCo}_{1-x}\text{Ni}_x\text{O}_{3-\delta}$ Perovskites in the Degradation of Rhodamine B

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Supporting Information

Table S1. Crystal space group, lattice parameters, crystal size, density, and fitting parameters from Rietveld refinement for all synthesized perovskites.

	$\text{LaCoO}_{3-\delta}$	$\text{LaCo}_{0.8}\text{Ni}_{0.2}\text{O}_{3-\delta}$	$\text{LaCo}_{0.6}\text{Ni}_{0.4}\text{O}_{3-\delta}$	$\text{LaCo}_{0.4}\text{Ni}_{0.6}\text{O}_{3-\delta}$	$\text{LaCo}_{0.2}\text{Ni}_{0.8}\text{O}_{3-\delta}$
Space group	$R\bar{3}c$ (167)	$R\bar{3}c$ (167)	$R\bar{3}c$ (167)	$R\bar{3}c$ (167)	$R\bar{3}c$ (167)
Volume [\AA^3]	335.736±0.009	337.974±0.007	339.228±0.007	339.516±0.016	339.651±0.009
a,b [\AA]	5.4420±0.0001	5.4560±0.0001	5.4633±0.0001	5.4618±0.0002	5.4646±0.0001
c [\AA]	13.0902±0.0002	13.1099±0.0001	13.1236±0.0001	13.1418±0.0003	13.1336±0.0002
Crystal size [nm]	290	250	238	160	153
microstrain	885	950	1148	2334	1284
R_w	3.39	3.397	3.33	5.25	3.79
GOF	1.00	1.00	0.93	1.28	1.01

Table S2. Atomic positions and thermal parameters of $\text{LaCoO}_{3-\delta}$ and $\text{LaCo}_{0.2}\text{Ni}_{0.8}\text{O}_{3-\delta}$ from Rietveld refinements. Differences compared to that in the ICDD database is shown in brackets.

Composition	Element	x	y	z	U_{iso}
$\text{LaCoO}_{3-\delta}$	La	0.00000	0.00000	0.25000	0.00677
	Co	0.00000	0.00000	0.00000	0.00414
	O	0.44701 (0.444)	0.00000	0.75000	0.00124
$\text{LaCo}_{0.2}\text{Ni}_{0.8}\text{O}_{3-\delta}$	La	0.00000	0.00000	0.25000	0.01000

Co	0.00000	0.00000	0.00000	0.01000
Ni	0.00000	0.00000	0.00000	0.01000
O	0.53876 (0.54946)	0.00000	0.25000	0.02813

Table S3. Amounts of chemicals used for synthesizing of each perovskite composition.

Composition	$\text{La}(\text{NO}_3)_3 \cdot 6\text{H}_2\text{O}$ [g]	$\text{Co}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ [g]	$\text{Ni}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ [g]	$\text{C}_6\text{H}_8\text{O}_7$ [g]	NH_4NO_3 [g]
$\text{LaCoO}_{3-\delta}$	4.330	2.910	-	7.685	9.205
$\text{LaCo}_{0.8}\text{Ni}_{0.2}\text{O}_{3-\delta}$	4.330	2.328	0.582	7.685	9.205
$\text{LaCo}_{0.6}\text{Ni}_{0.4}\text{O}_{3-\delta}$	4.330	1.746	1.163	7.685	9.205
$\text{LaCo}_{0.4}\text{Ni}_{0.6}\text{O}_{3-\delta}$	4.330	1.164	1.745	7.685	9.205
$\text{LaCo}_{0.2}\text{Ni}_{0.8}\text{O}_{3-\delta}$	4.330	0.582	2.326	7.685	9.205

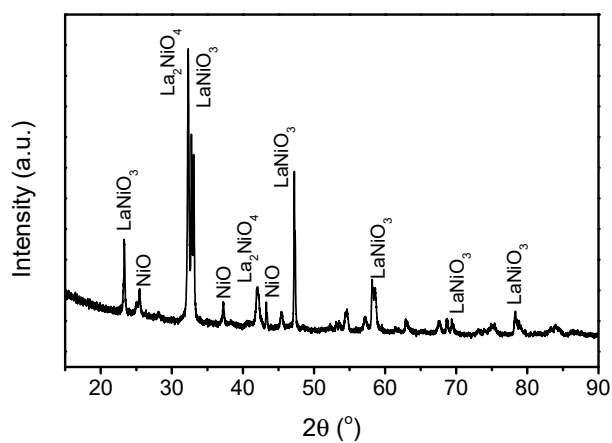


Figure S1. X-ray diffractogram of synthesized LaNiO_3 containing impurities.

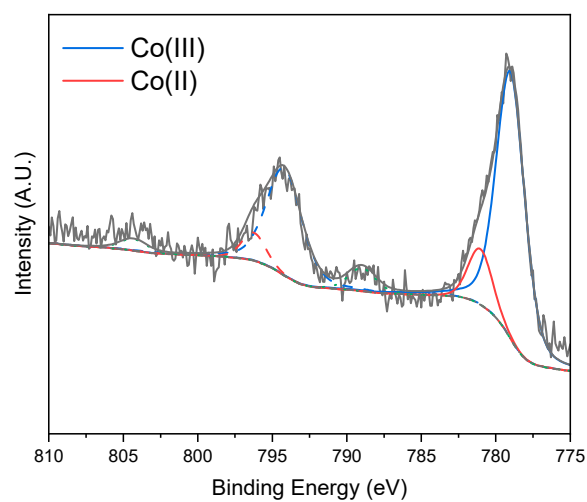


Figure S2. Fitted Co 2p region of $\text{LaCoO}_{3-\delta}$. Bold line Co 2p 3/2, dashed line Co 2p 1/2; green dotted line Co satellites.

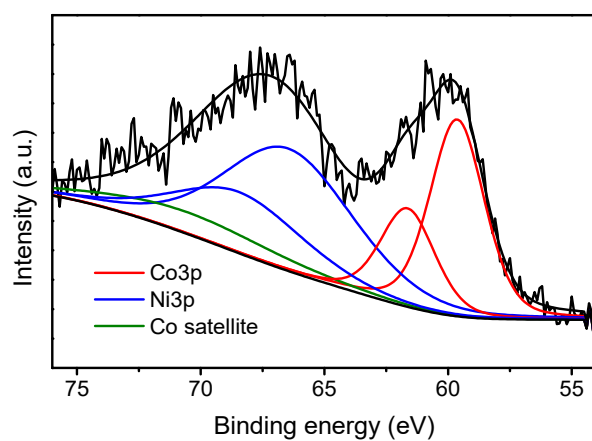


Figure S3. Fitted Co 2p, Ni 2p XPS region of $\text{LaCo}_{0.6}\text{Ni}_{0.4}\text{O}_{3-\delta}$.

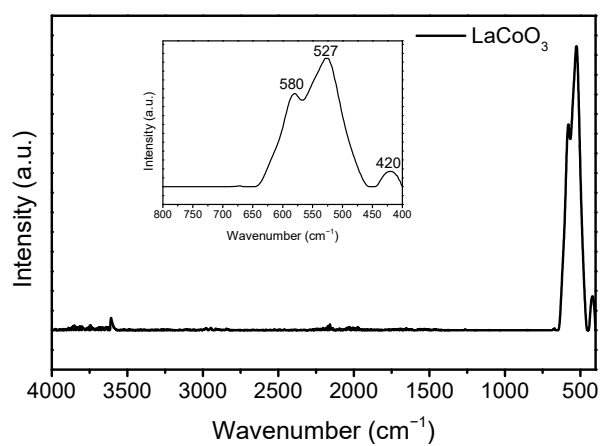


Figure S4. ATR-FTIR of $\text{LaCoO}_{3-\delta}$. Inset shows a zoom of the main signals.

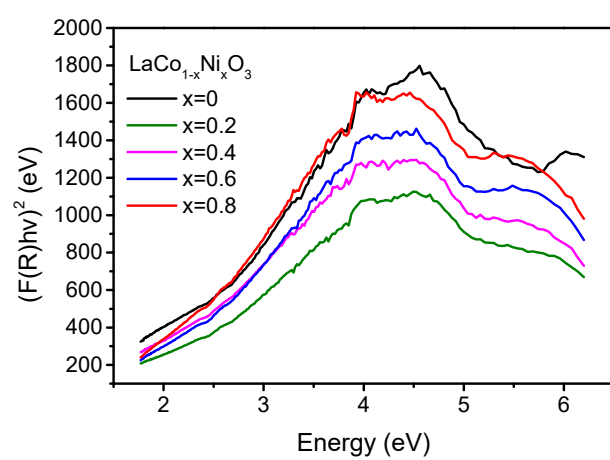


Figure S5. Kubelka-Munk plots for determination of the energy band gap.

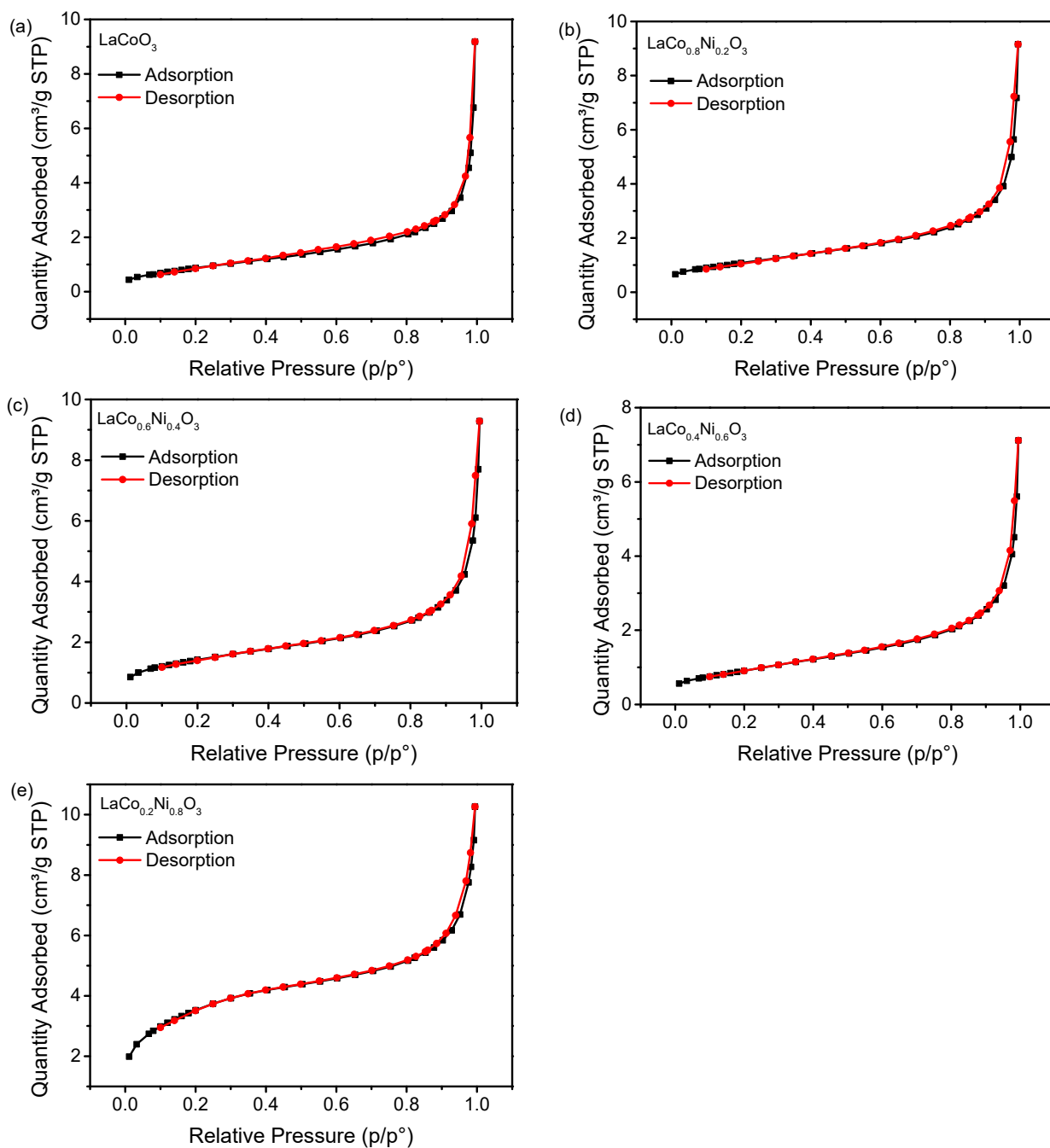


Figure S6. N_2 adsorption and desorption isotherms for the synthesized perovskites (a) $\text{LaCoO}_{3-\delta}$, (b) $\text{LaCo}_{0.8}\text{Ni}_{0.2}\text{O}_{3-\delta}$, (c) $\text{LaCo}_{0.6}\text{Ni}_{0.4}\text{O}_{3-\delta}$, (d) $\text{LaCo}_{0.4}\text{Ni}_{0.6}\text{O}_{3-\delta}$, and (e) $\text{LaCo}_{0.2}\text{Ni}_{0.8}\text{O}_{3-\delta}$.

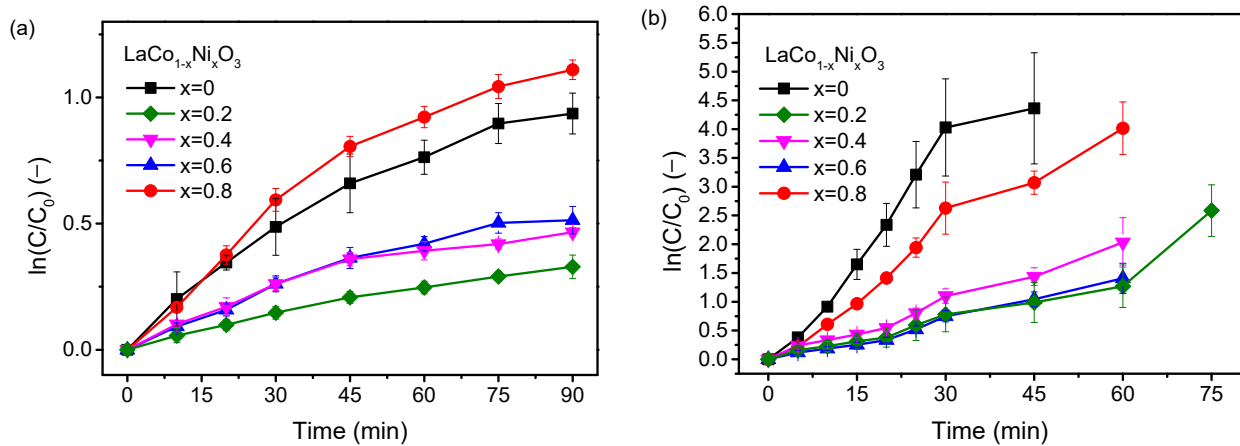


Figure S7. Degradation of rhodamine B at perovskite concentrations of (a) 100 mg L^{-1} and (b) 500 mg L^{-1} .

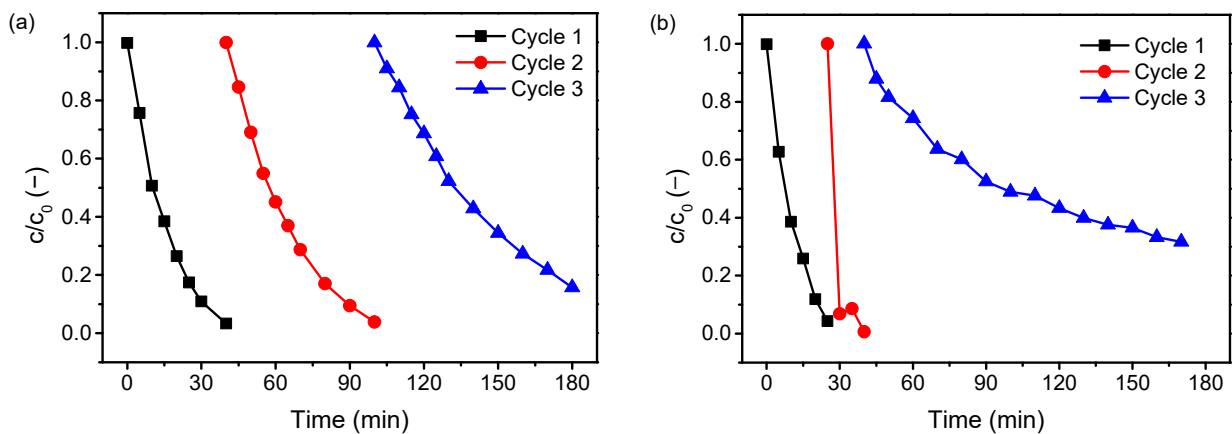


Figure S8. Stability of (a) $\text{LaCoO}_{3-\delta}$ and (b) $\text{LaCo}_{0.2}\text{Ni}_{0.8}\text{O}_{3-\delta}$ during 3 cycles of catalytic degradation of rhodamine B at 25°C .

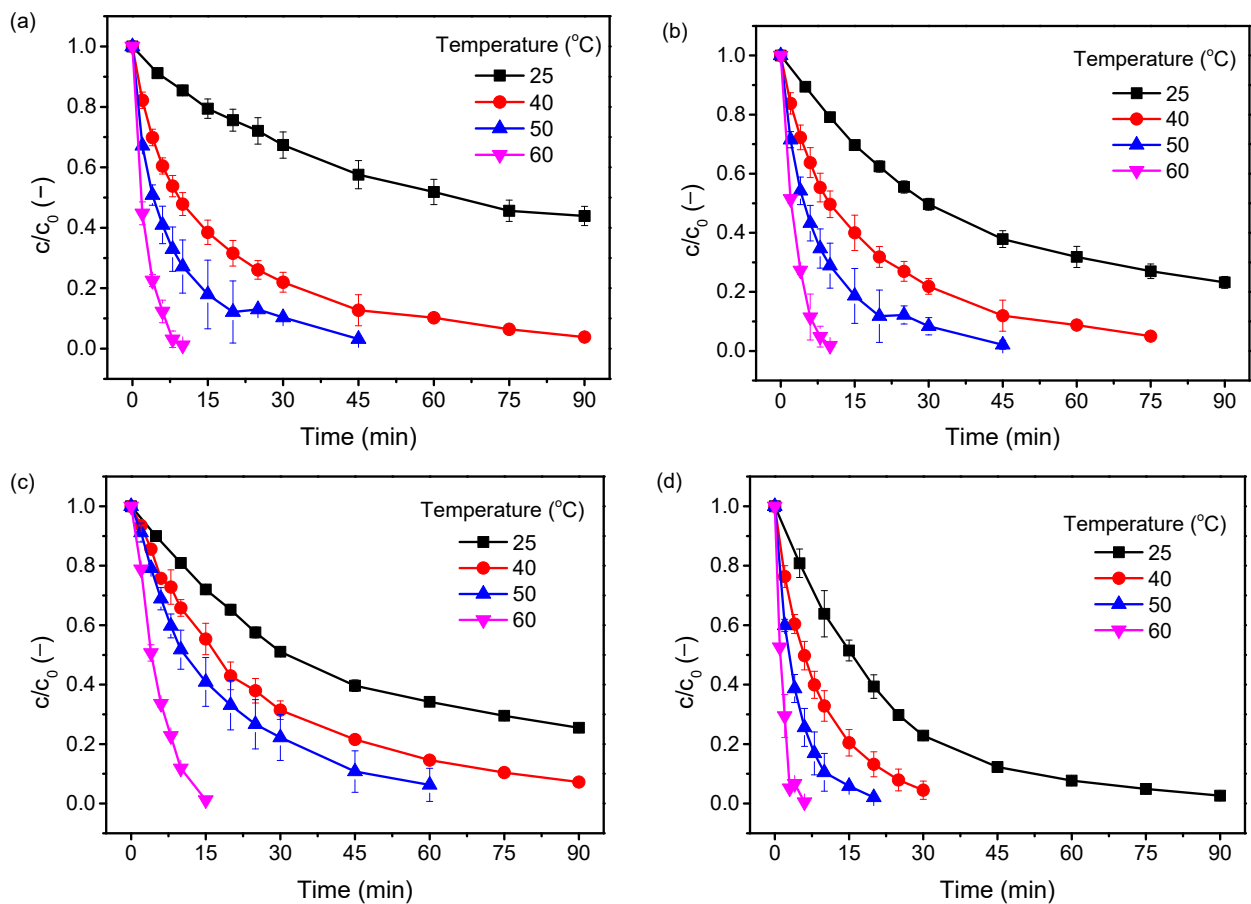


Figure S9. Temperature effect on catalytic activity for (a) $\text{LaCo}_{0.8}\text{Ni}_{0.2}\text{O}_{3-\delta}$, (b) $\text{LaCo}_{0.6}\text{Ni}_{0.4}\text{O}_{3-\delta}$, (c) $\text{LaCo}_{0.4}\text{Ni}_{0.6}\text{O}_{3-\delta}$, and (d) $\text{LaCo}_{0.2}\text{Ni}_{0.8}\text{O}_{3-\delta}$.