

Supplementary materials

Effect of Al and Fe Doping on the Electrochemical Behavior of $\text{Li}_{1.2}\text{Ni}_{0.133}\text{Mn}_{0.534}\text{Co}_{0.133}\text{O}_2$ Li-Rich Cathode Material

Anna Medvedeva ^{1,*}, Elena Makhonina ¹, Lidia Pechen ¹, Yury Politov ¹, Aleksander Rumyantsev ², Yury Koshtyal ², Alexander Goloveshkin ³, Konstantin Maslakov ⁴ and Igor Eremenko ^{1,*}

¹ Kurnakov Institute of General and Inorganic Chemistry of the Russian Academy of Sciences, 31 Leninsky pr., 119991 Moscow, Russia

² Ioffe Institute of the Russian Academy of Sciences, 26 Politekhnicheskaya ul., 194021 St. Petersburg, Russia

³ A.N. Nesmeyanov Institute of Organoelement Compounds of the Russian Academy of Sciences, 28 Vavilova ul., 119334 Moscow, Russia

⁴ Department of Chemistry, Lomonosov Moscow State University, Leninskiye Gory, 1/3, 119991 Moscow, Russia

* Correspondence: anna.ev.medvedeva@gmail.com (A.M.); ilerem@igic.ras.ru (I.E.); Tel.: +7-495-952-07-87 (A.M.)

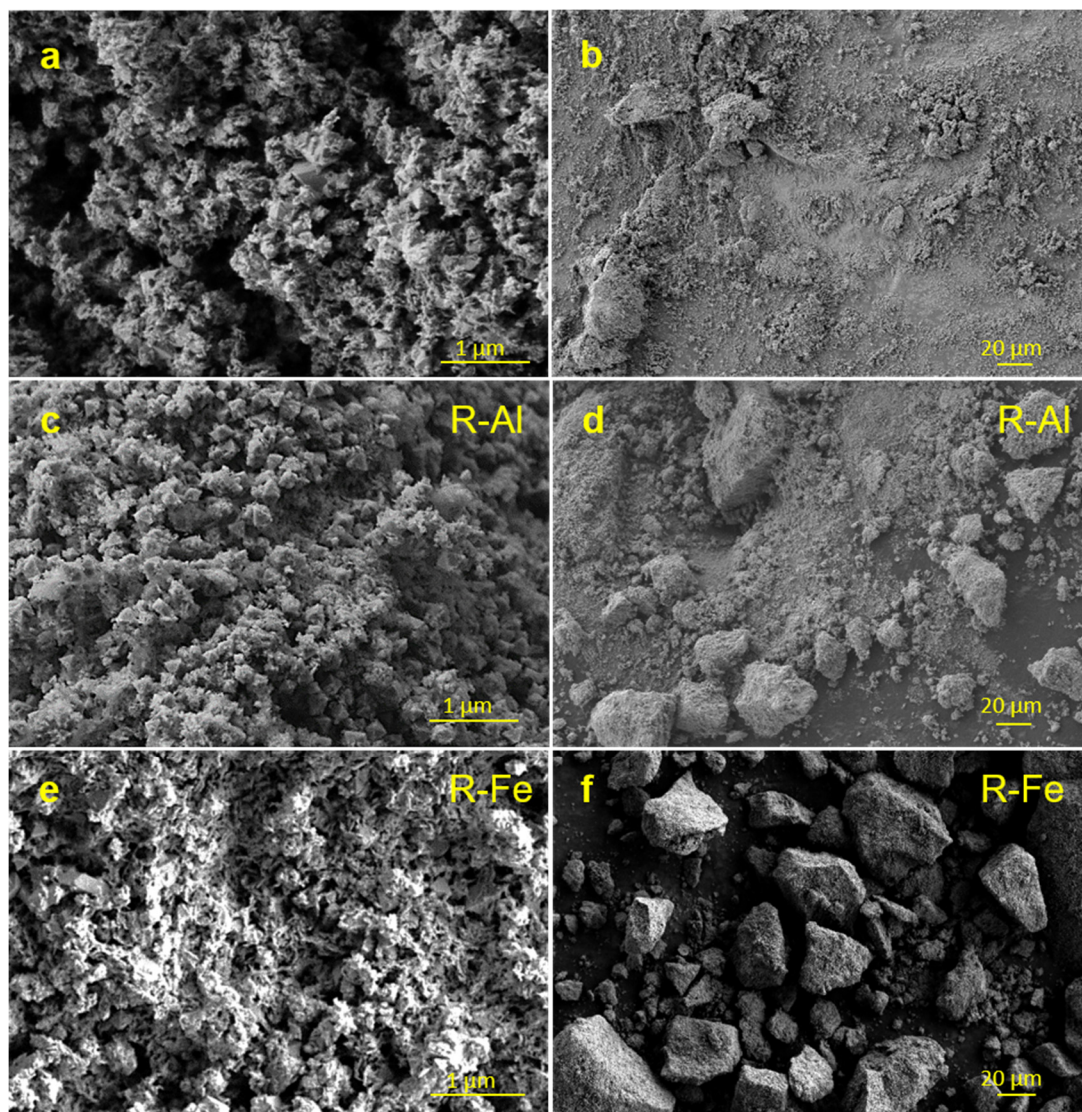


Figure S1. SEM micrographs of (a, b) R, (c, d) R – Al, and (e, f) R – Fe samples.

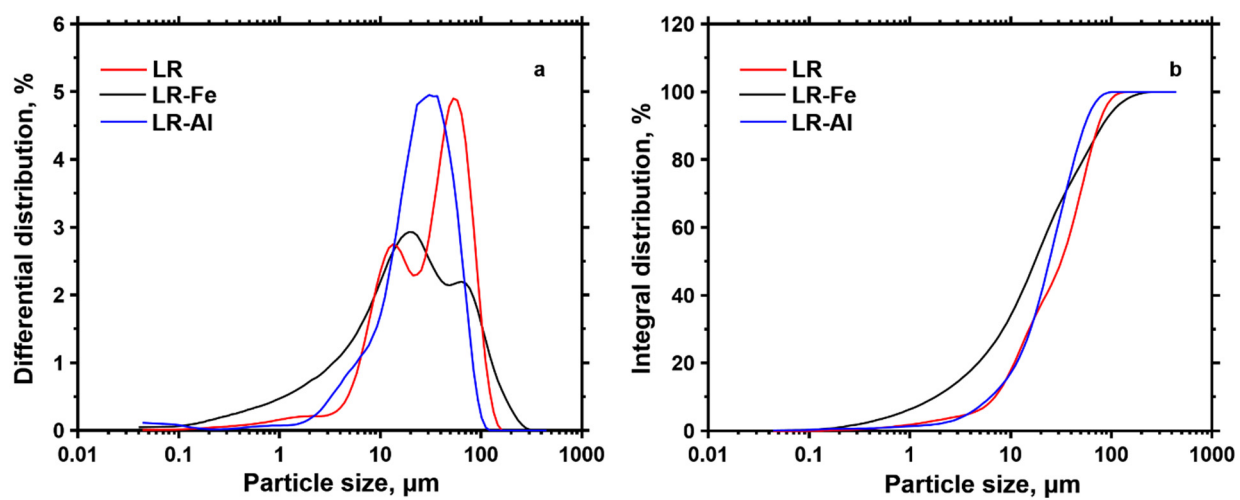


Figure S2. Differential and integral size distribution curves of agglomerates of the synthesized samples.

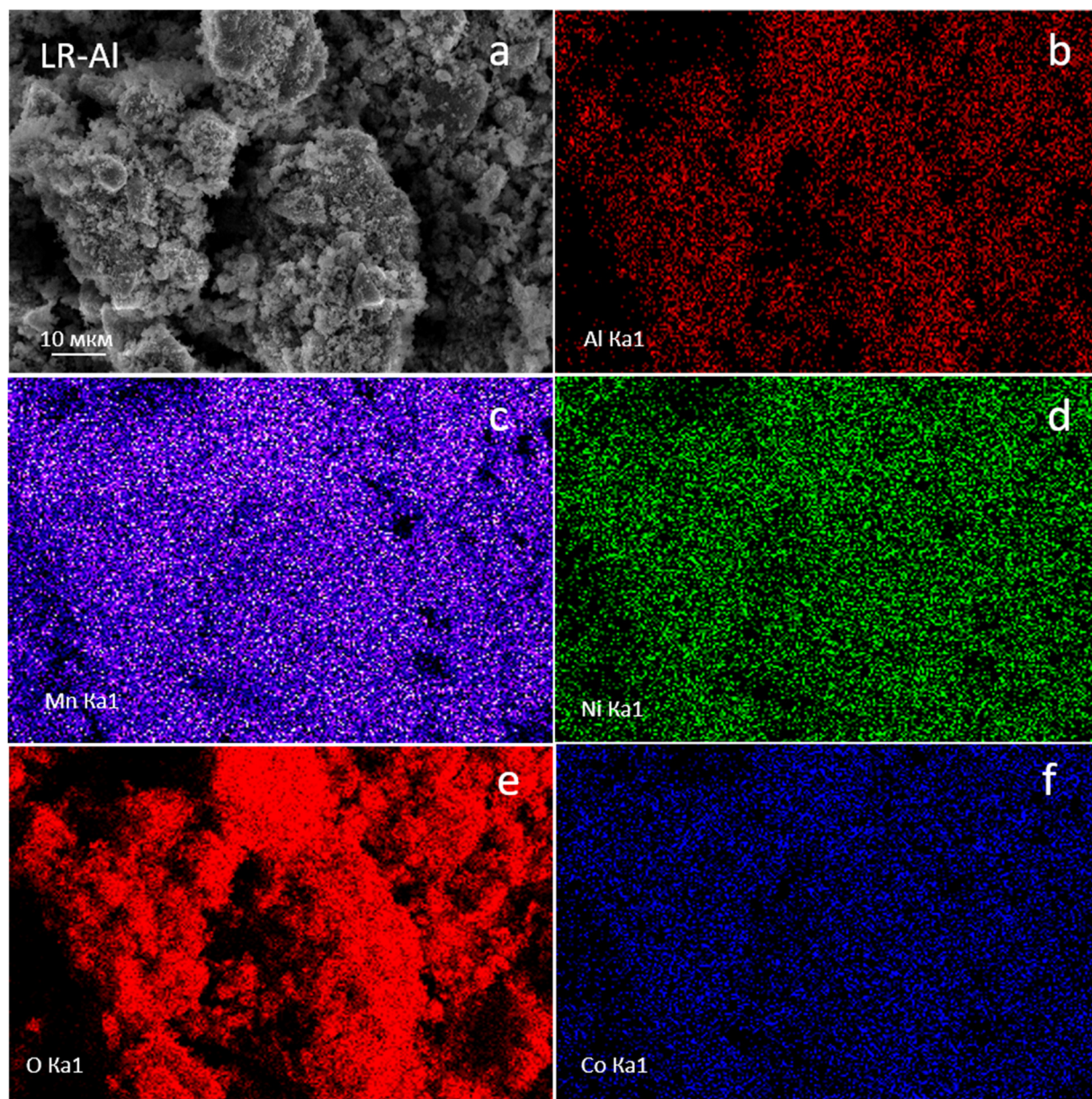


Figure S3. (a) SEM micrograph of LR – Al sample and (b-f) the element distribution maps: (b) Al, (c) Mn, (d) Ni, (e) O, and (f) Co.

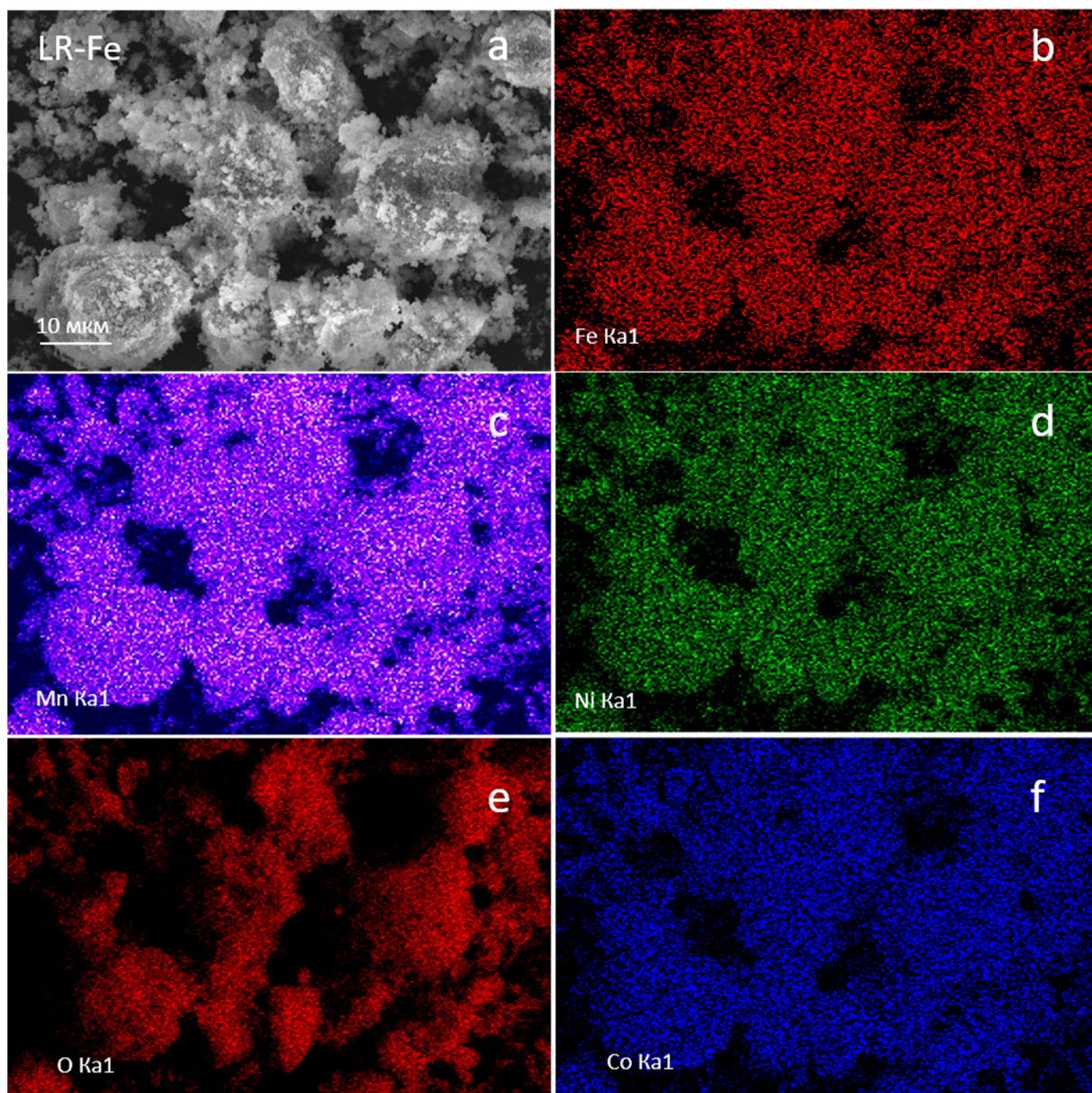


Figure S4. (a) SEM micrograph of LR – Fe sample and (b-f) element distribution maps: (b) Fe, (c) Mn, (d) Ni, (e) O, and (f) Co.

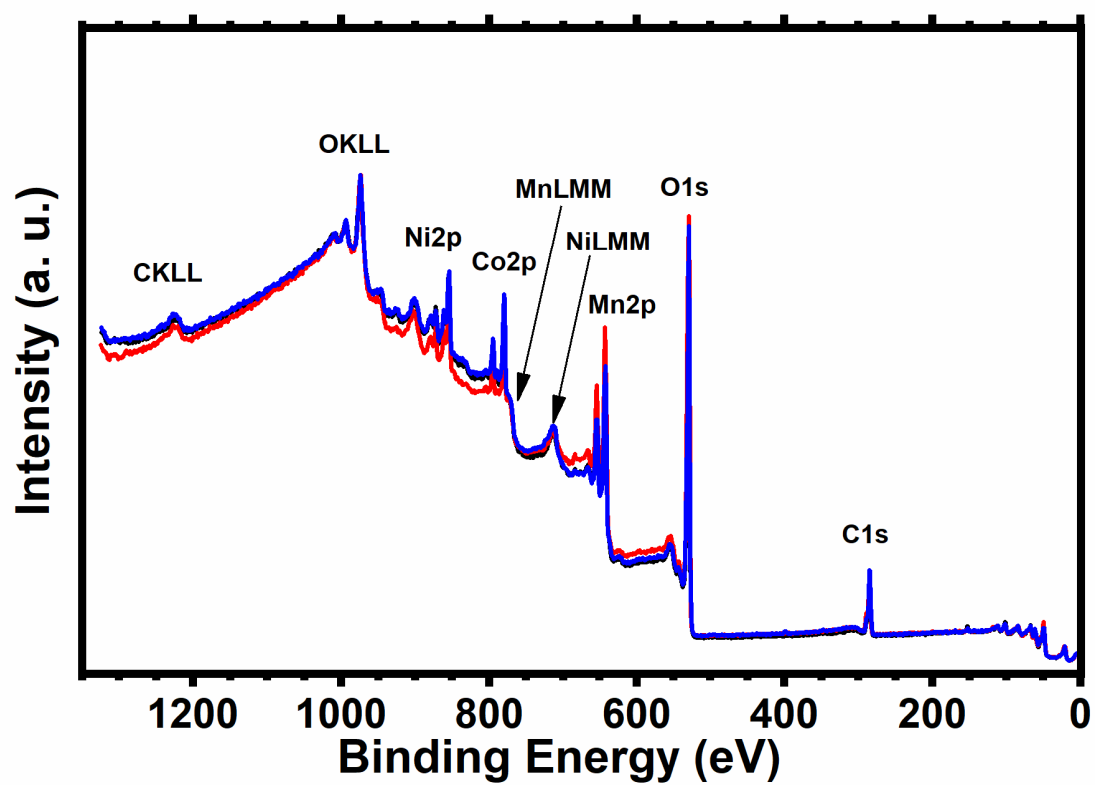


Figure S5. Survey XPS spectra of the samples LR, LR-Al and LR-Fe samples.

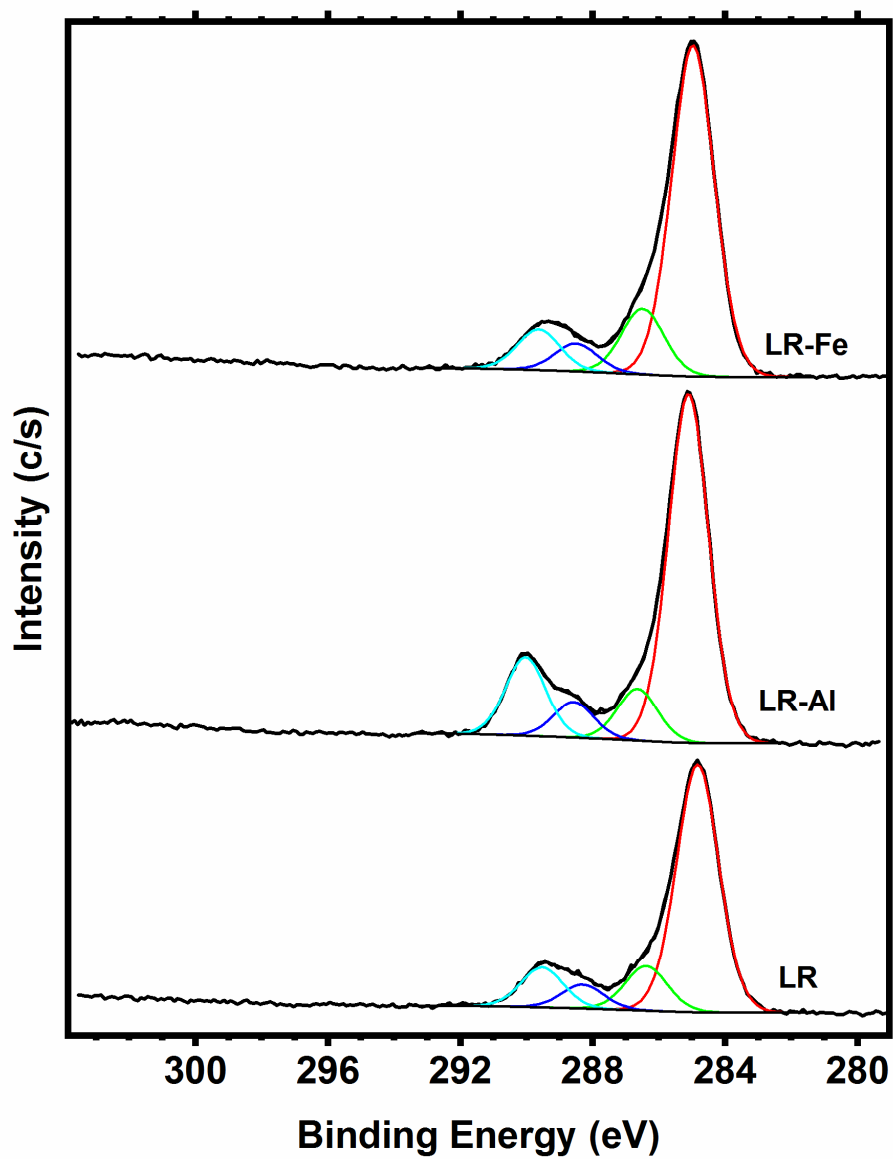


Figure S6. C1s spectra of LR, LR-Al and LR-Fe samples.

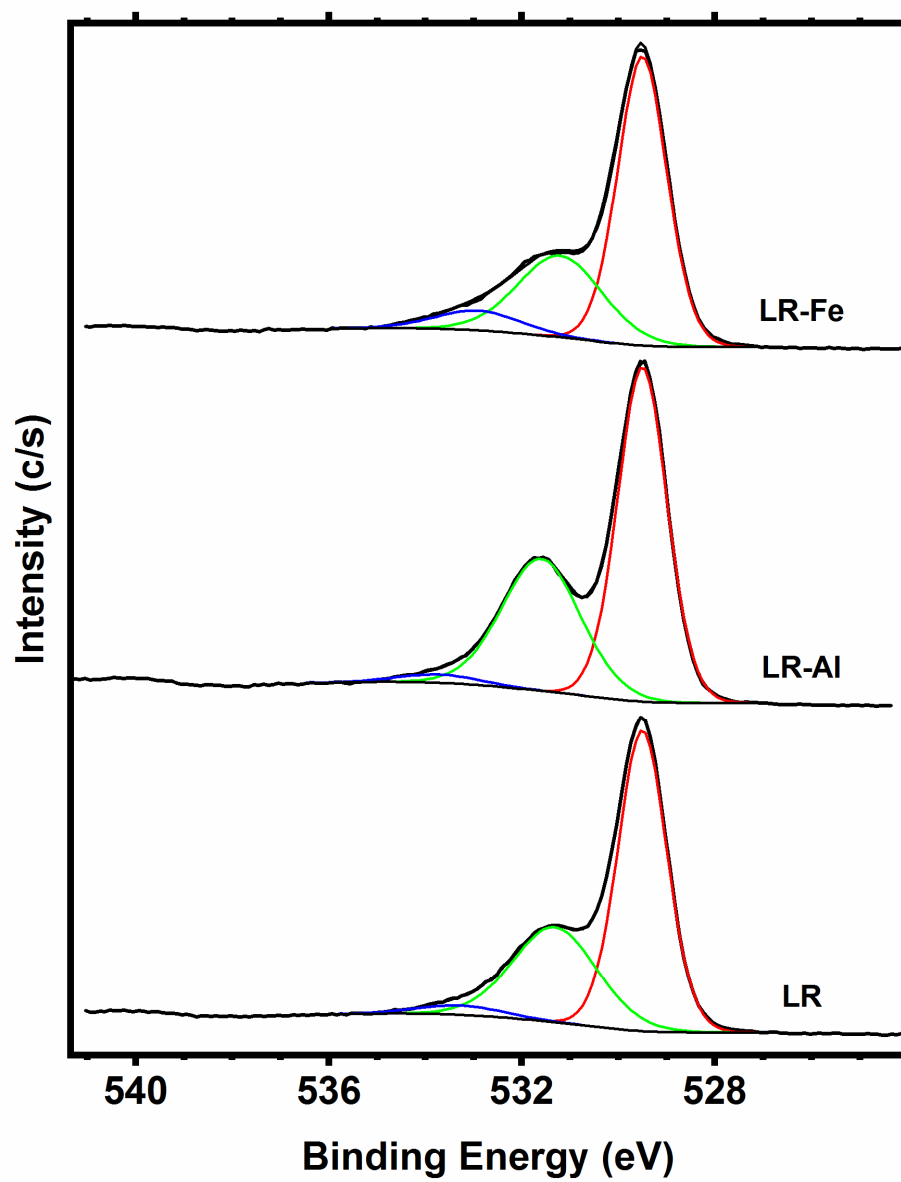


Figure S7. O1s spectra of LR, LR-Al and LR-Fe.

Table S1. Concentrations of elements on the surface of the studied samples (at %), calculated from the high-resolution XPS spectra

Samples	Ni	Co	Mn	O	C	Fe	Al
LR	6.2	4.9	11.8	55.6	21.5	–	–
LR-Al	4.7	2.9	11.8	54.9	25.1	–	0.6
LR-Fe	5.2	4.7	10.4	51.3	26.9	1.5	–

Table S2. Binding energies of the Co2p_{3/2} lines and the relative position of the satellite (Δ Co2p_{sat}) in the XPS spectra of the studied samples and reference cobalt compounds, eV.

Samples	Co2p _{3/2}	Δ Co2p _{sat}	Ref.
LR	780.0	9.6	
LR-Al	780.2	9.6	
LR-Fe	780.0	9.6	
ScCo _{0.95} Fe _{0.95} O ₃ (Co ³⁺)	780.2	10.2	[53]
Co(OH) ₂ (Co ²⁺)	781.2	5.0	[54]
LiCoO ₂ (Co ³⁺)	780.2	9.9	[55]
LiNi _{0.4} Mn _{0.4} Co _{0.2} O ₂ (Co ³⁺)	780.2	9.5	[55]
LiCoO ₂ (Co ³⁺)	779.6	8.6	[56]
Li _{0.5} Co _{0.5} Ni _{0.5} O ₂ (Co ³⁺)	779.4	9.0	[56]

Table S3. Binding energies of Mn2p_{3/2} and Mn3s XPS spectra, relative satellite position (Δ Mn2p_{sat}) in Mn2p_{1/2} XPS spectra, splitting (Δ Mn3s) of Mn3s XPS spectra of the studied samples and reference manganese oxides, eV.

Samples	Mn2p _{3/2}	Δ Mn2p _{sat}	Mn3s	Δ Mn3s	O1s	Ref.
LR	642.1	11.4	84.6	4.4	529.5	
LR-Al	642.1	11.4	84.6	4.5	529.5	
LR-Fe	642.1	11.4	84.7	4.3	529.5	
MnO (Mn ²⁺)	640.8	~6.0	83.1	6.1	529.6	[57,58]
Mn ₂ O ₃ (Mn ³⁺)	641.8	10.1	83.8	5.4	530.0	[59]
MnO ₂ (Mn ⁴⁺)	642.4	11.8	84.7	4.4	529.6	[60]