

Supporting Information

Raman Diagnostics of Cathode Materials for Li-Ion Batteries Using Multi-Wavelength Excitation

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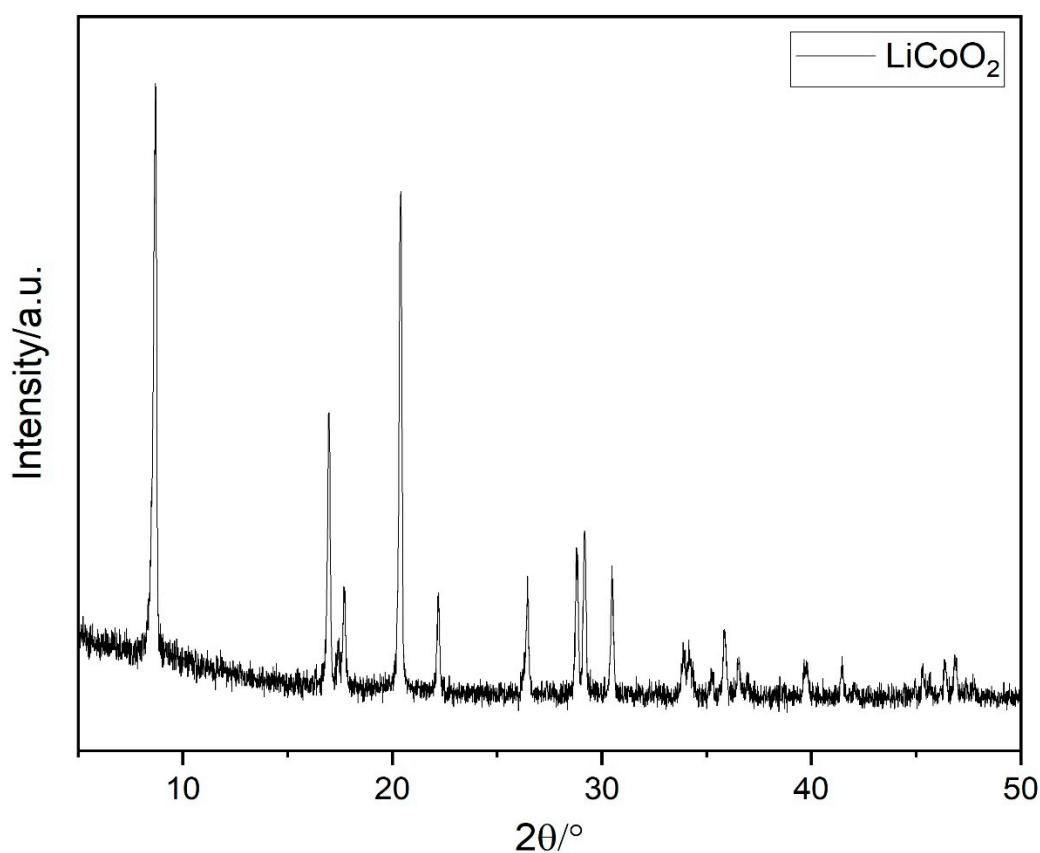


Figure S1. XRD results (Mo $K_{\alpha 1}$) of the prepared LiCoO_2 . The refined a and c parameters are 2.8147(2) Å and 14.0437(9) Å, respectively.

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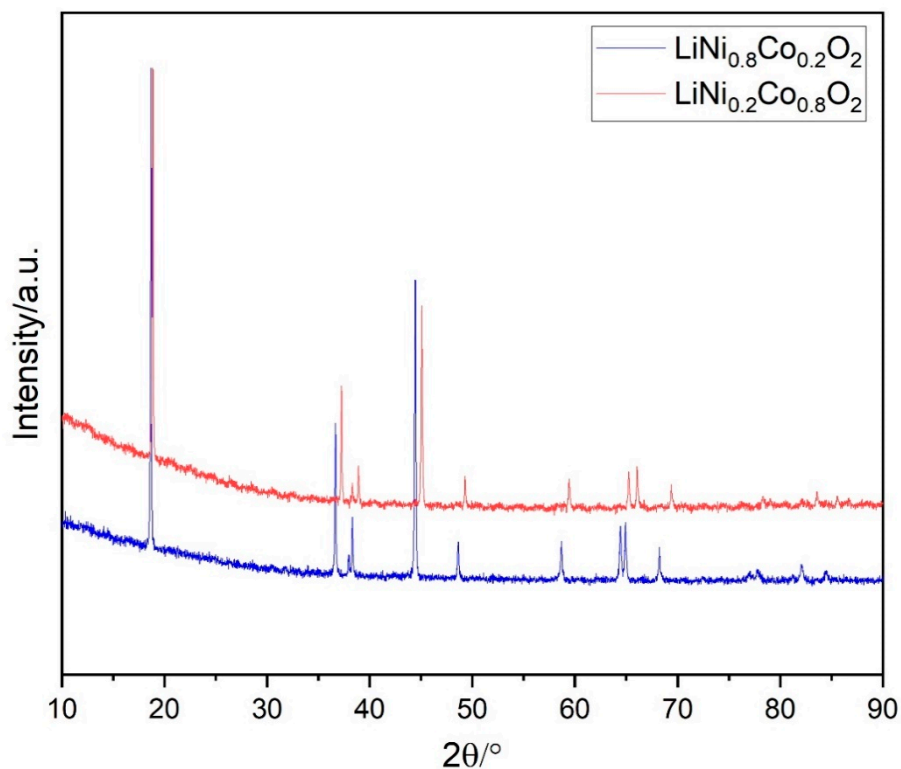


Figure S2. XRD results (Cu $K_{\alpha 1}$) of the prepared $\text{LiNi}_{0.2}\text{Co}_{0.8}\text{O}_2$ (red) and $\text{LiNi}_{0.8}\text{Co}_{0.2}\text{O}_2$ (blue). The refined a and c parameters of $\text{LiNi}_{0.2}\text{Co}_{0.8}\text{O}_2$ are 2.83369(5) Å and 14.01716(7) Å, and those of $\text{LiNi}_{0.8}\text{Co}_{0.2}\text{O}_2$ are 2.86810(6) Å and 14.1952(7) Å, respectively.

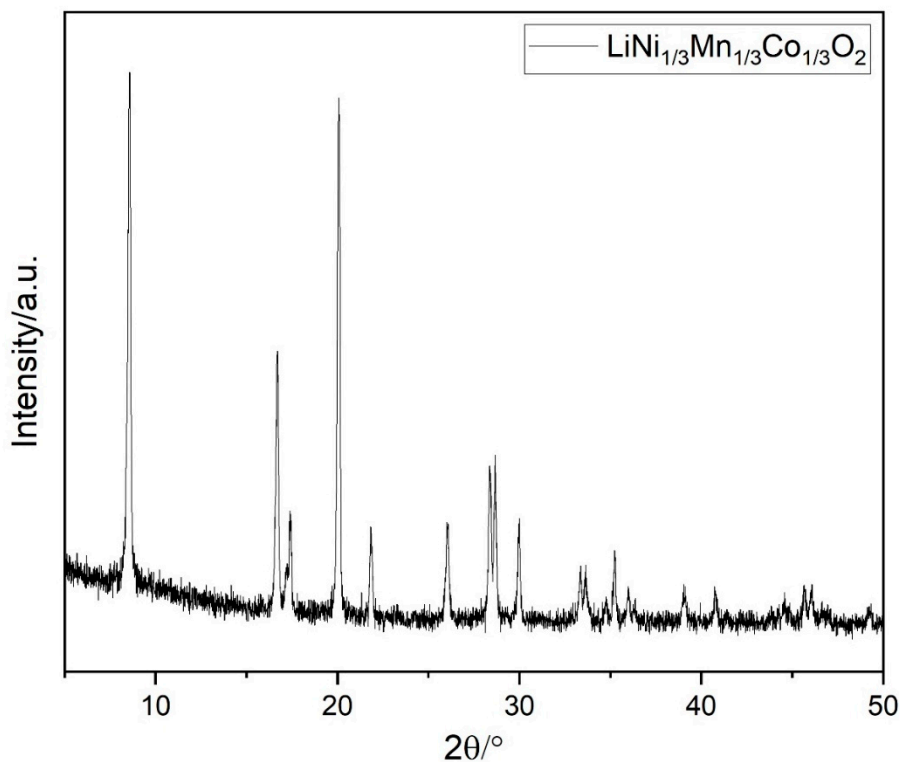


Figure S3. XRD results (Cu $K_{\alpha 1}$) of the prepared $\text{LiNi}_{0.2}\text{Co}_{0.8}\text{O}_2$ (red) and $\text{LiNi}_{0.8}\text{Co}_{0.2}\text{O}_2$ (blue). The refined a and c parameters of $\text{LiNi}_{0.2}\text{Co}_{0.8}\text{O}_2$ are 2.83369(5) Å and 14.01716(7) Å, and those of $\text{LiNi}_{0.8}\text{Co}_{0.2}\text{O}_2$ are 2.86810(6) Å and 14.1952(7) Å, respectively.

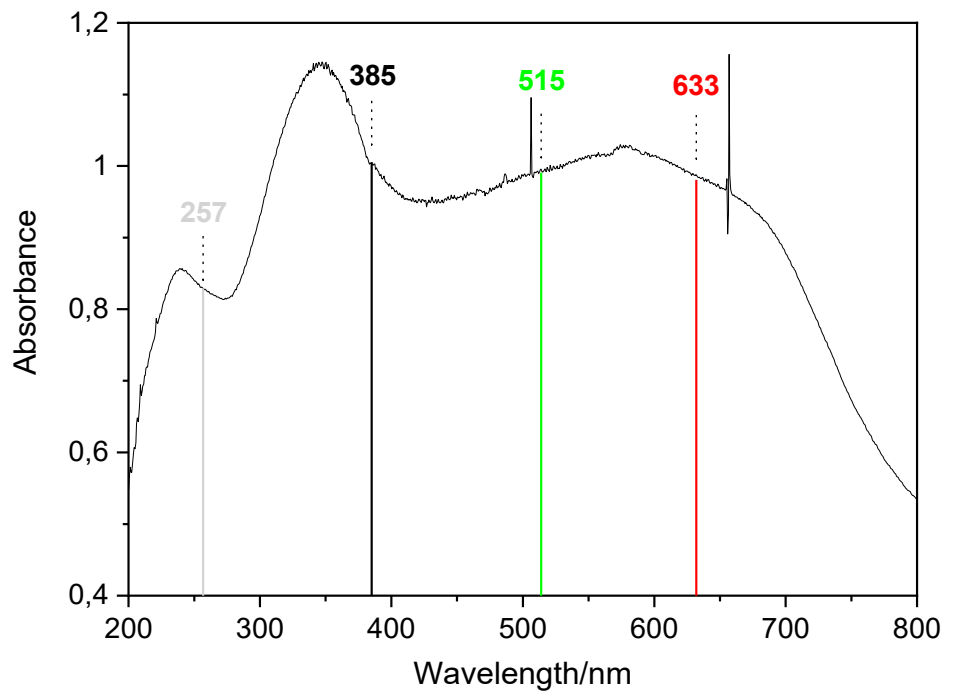
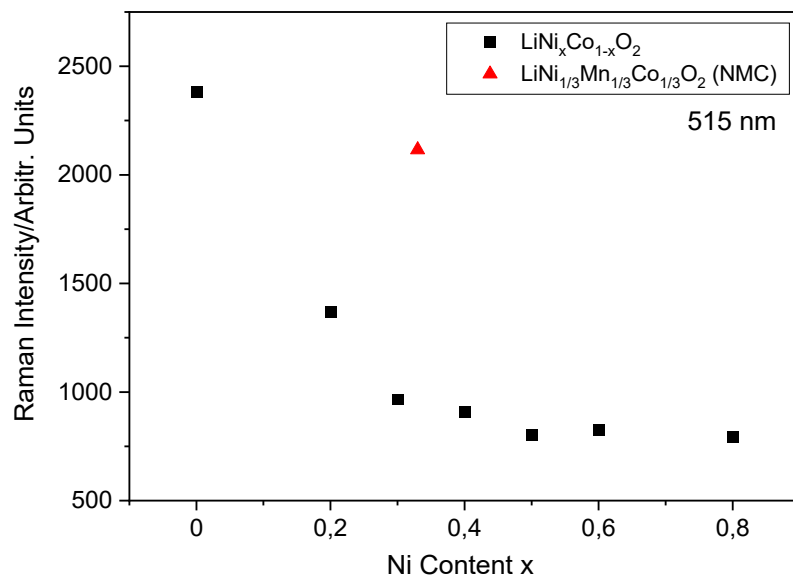


Figure S4. UV-Vis spectrum of LiCoO₂ together with the used excitation wavelengths (257, 385, 515, and 633 nm).

Table S1. Direct products for point group D_{3d} leading to Raman-active modes.

	A _{1g}	A _{2g}	E _g	A _{1u}	A _{2u}	E _u
A _{1g}	A _{1g}		E _g			
A _{2g}		A _{1g}	E _g			
E _g	E _g	E _g	A _{1g} ⊕ A _{2g} ⊕ E _g			
A _{1u}				A _{1g}		E _g
A _{2u}					A _{1g}	E _g
E _u				E _g	E _g	A _{1g} ⊕ A _{2g} ⊕ E _g



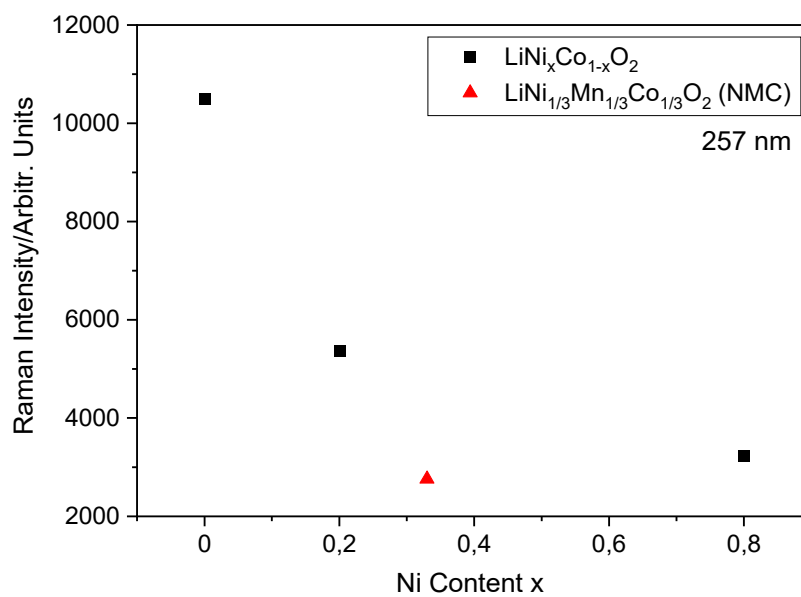


Figure S5. Raman intensity of the A_{1g} mode of LiCoO_2 , $\text{LiNi}_x\text{Co}_{1-x}\text{O}_2$ and $\text{LiNi}_{1/3}\text{Mn}_{1/3}\text{Co}_{1/3}\text{O}_2$ (NMC) as a function of the Nickel content x for 515 nm (top) und 257 nm (bottom) excitation.

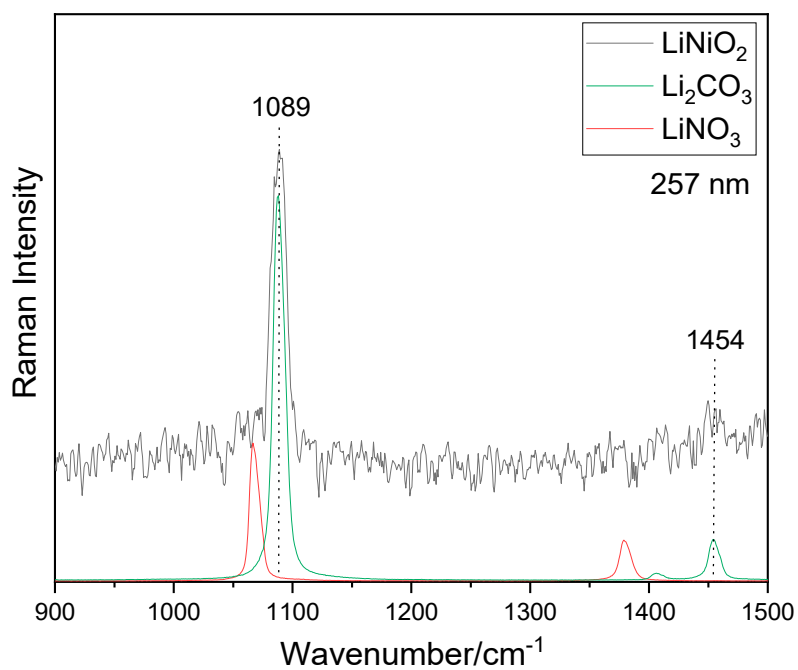


Figure S6. Raman spectra of LiNiO_2 and reference compounds at 257 nm excitation. Spectra were offset for clarity.