Supporting Information

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

Marcel Heber, Kathrin Hofmann and Christian Hess *

Eduard-Zintl-Institute for Inorganic and Physical Chemistry, Technical University of Darmstadt,
Alarich-Weiss-Str. 8, 64287 Darmstadt, Germany; Marcel.Heber@web.de (M.H.); kathrin.hofmann@tu-darmstadt.de (K.H.)
* Correspondence: christian.hess@tu-darmstadt.de; Tel.: +49-6151-16-21975; Fax: +49-6151-16-21979

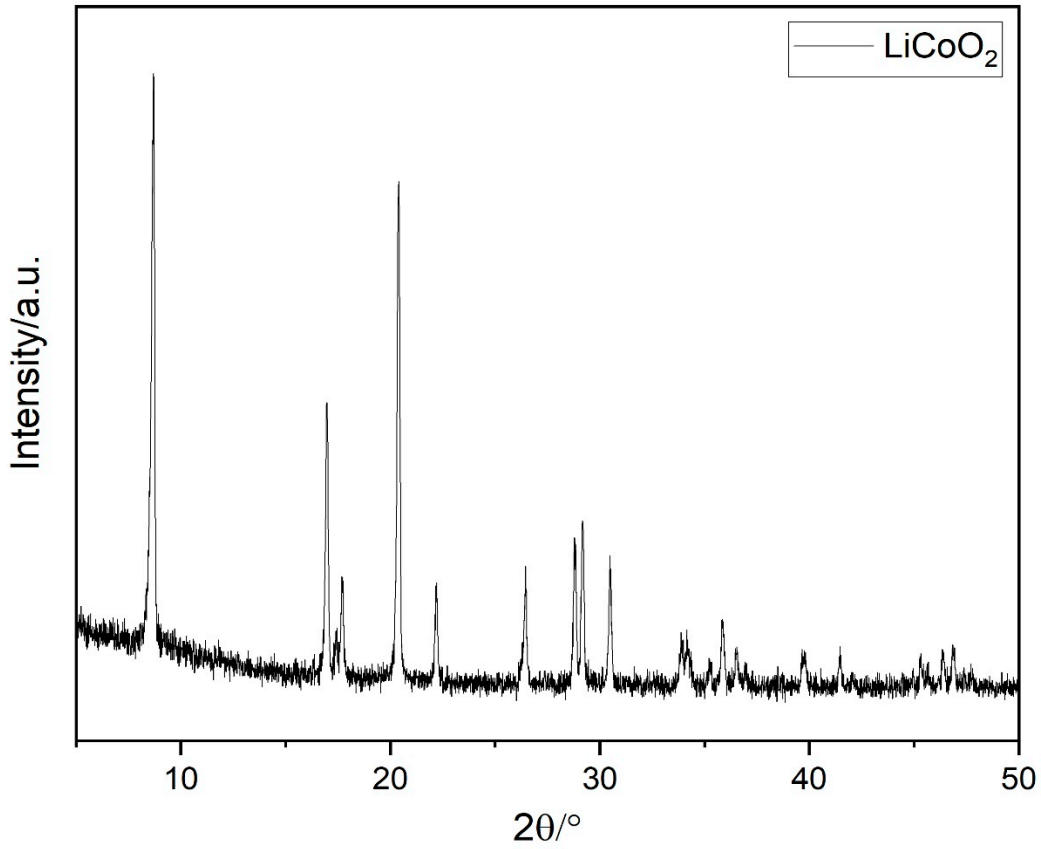


Figure S1. XRD results (Mo $K_{\alpha 1}$) of the prepared $LiCoO_2$. The refined a and c parameters are 2.8147(2) Å and 14.0437(9) Å, respectively.

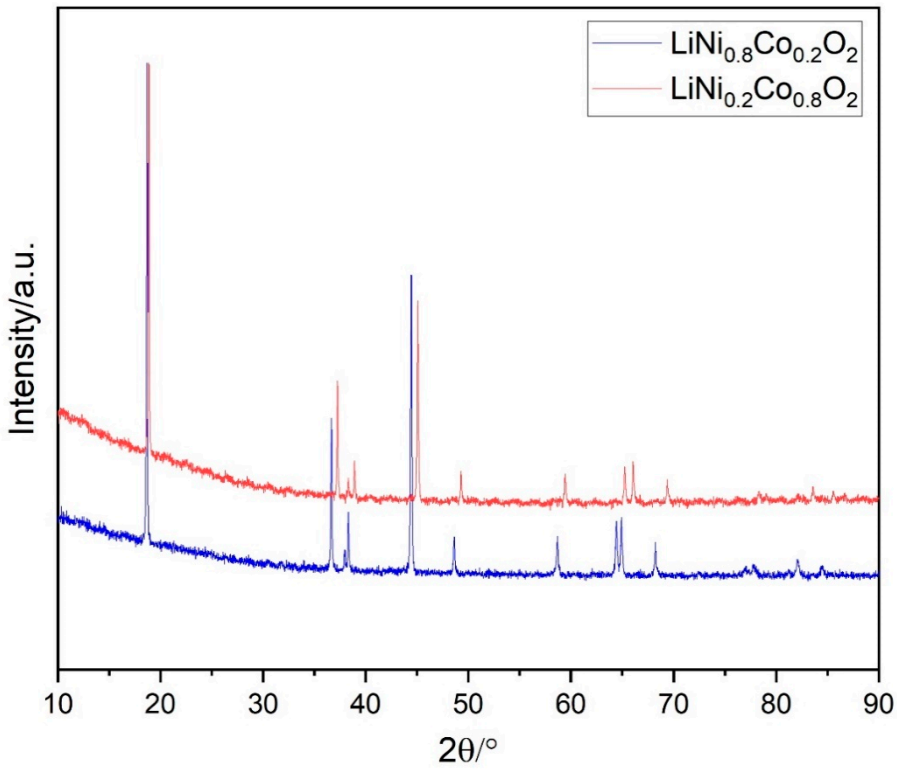


Figure S2. XRD results (Cu $K_{\alpha 1}$) of the prepared $LiNi_{0.2}Co_{0.8}O_2$ (red) and $LiNi_{0.8}Co_{0.2}O_2$ (blue). The refined a and c parameters of $LiNi_{0.2}Co_{0.8}O_2$ are 2.83369(5) Å and 14.01716(7) Å, and those of $LiNi_{0.8}Co_{0.2}O_2$ are 2.86810(6) Å and 14.1952(7) Å, respectively.

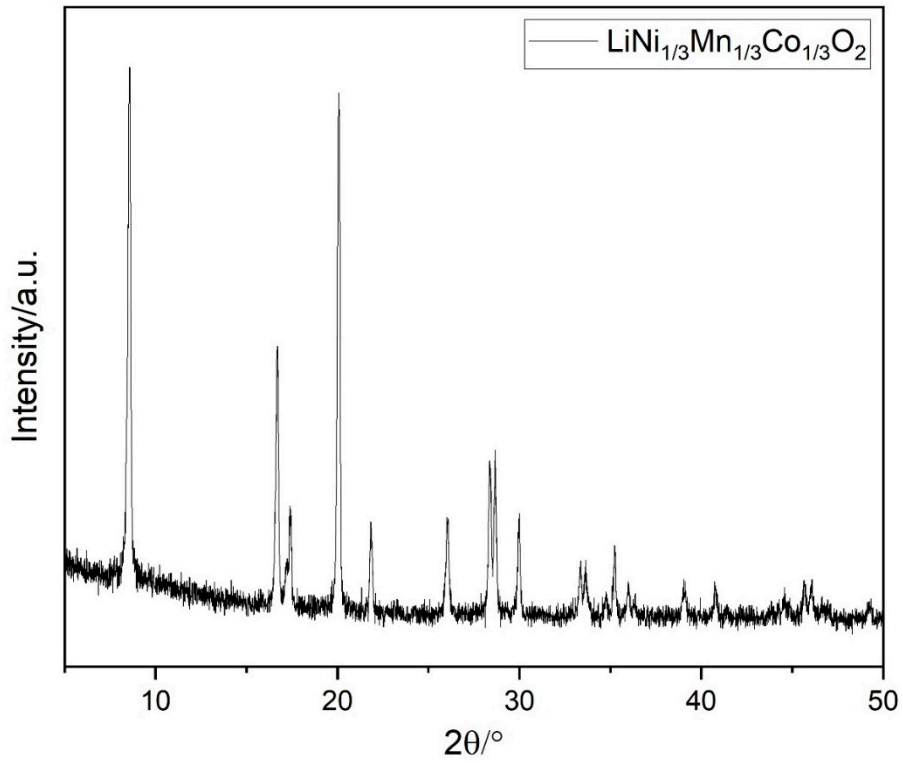


Figure S3. XRD results (Cu $K_{\alpha 1}$) of the prepared $LiNi_{0.2}Co_{0.8}O_2$ (red) and $LiNi_{0.8}Co_{0.2}O_2$ (blue). The refined a and c parameters of $LiNi_{0.2}Co_{0.8}O_2$ are 2.83369(5) Å and 14.01716(7) Å, and those of $LiNi_{0.8}Co_{0.2}O_2$ are 2.86810(6) Å and 14.1952(7) Å, respectively.

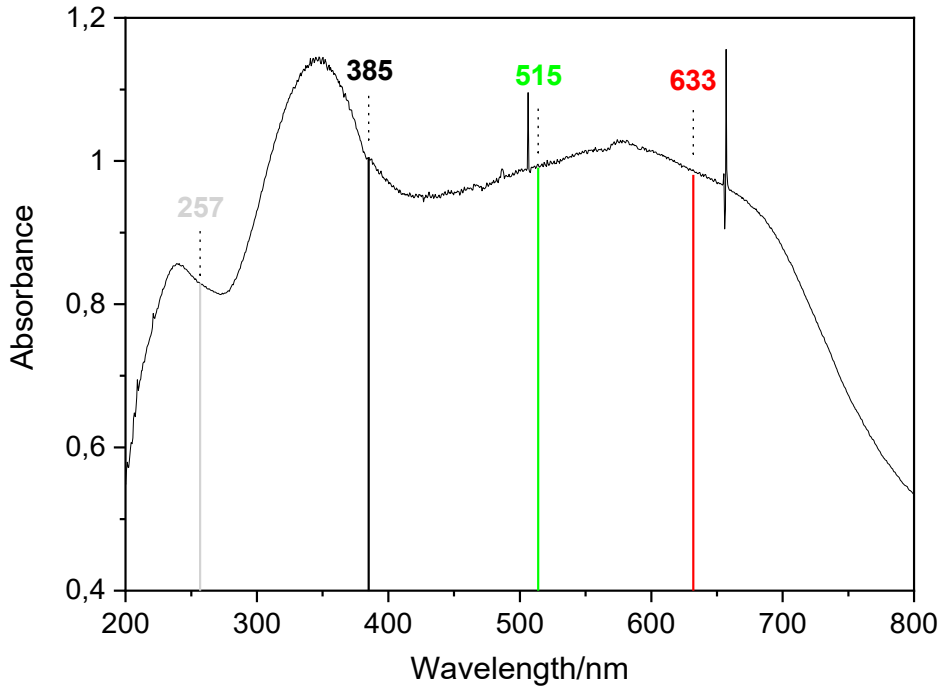
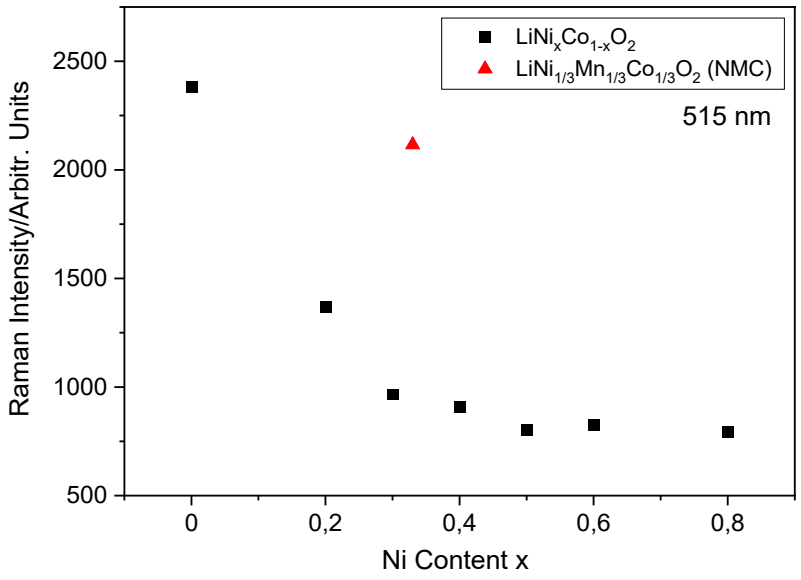


Figure S4. UV-Vis spectrum of $LiCoO_2$ together with the used excitation wavelengths (257, 385, 515, and 633 nm).

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

	$\mathbf{A_{1g}}$	$\mathbf{A_{2g}}$	$\mathbf{E_g}$	$\mathbf{A_{1u}}$	$\mathbf{A_{2u}}$	$\mathbf{E_u}$
A_{1g}	A_{1g}		E_g			
A_{2g}		A_{1g}	E_g			
E_g	E_g	E_g	$A_{1g} \oplus A_{2g} \oplus E_g$			
A_{1u}				A_{1g}		E_g
A_{2u}					A_{1g}	E_g
E_u				E_g	E_g	$A_{1g} \oplus A_{2g} \oplus E_g$



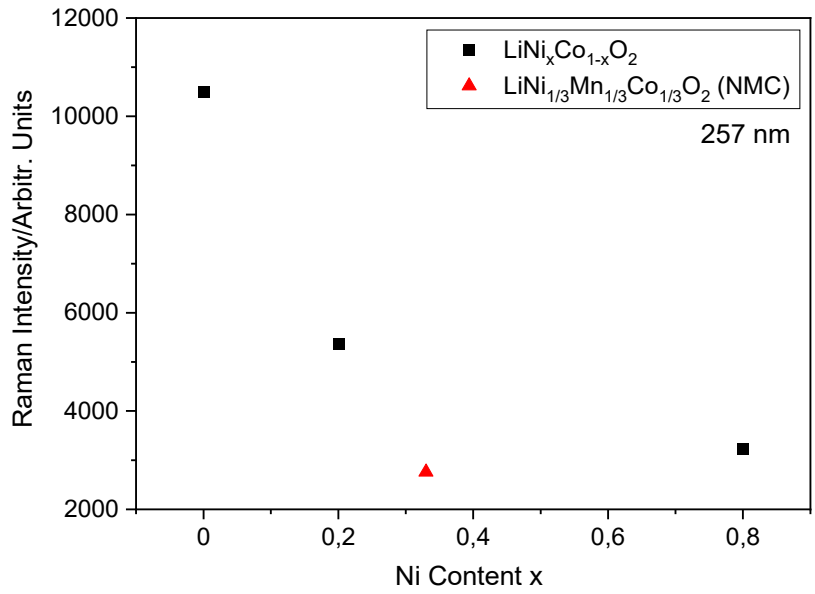


Figure S5. Raman intensity of the A_{1g} mode of $LiCoO_2$, $LiNi_xCo_{1-x}O_2$ and $LiNi_{1/3}Mn_{1/3}Co_{1/3}O_2$ (NMC) as a function of the Nickel content x for 515 nm (top) und 257 nm (bottom) excitation.

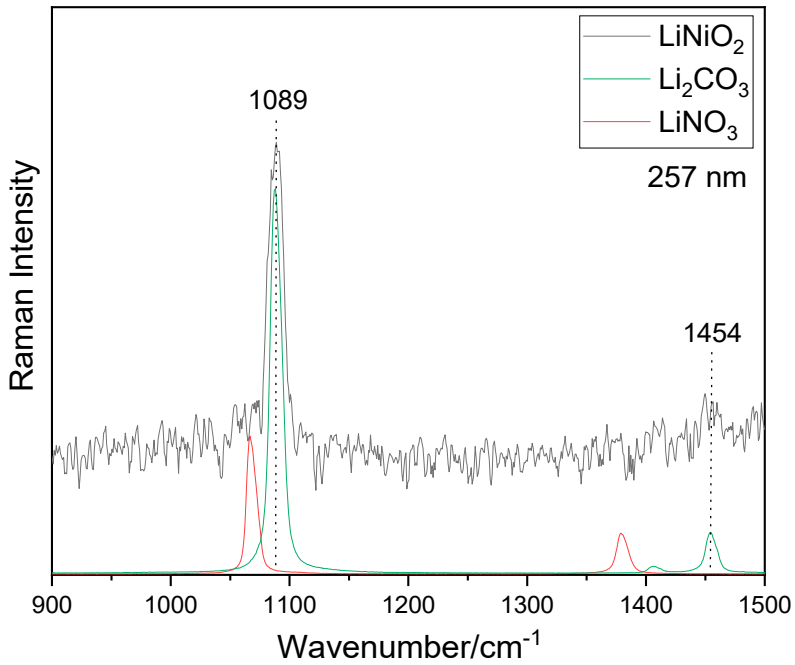


Figure S6. Raman spectra of $LiNiO_2$ and reference compounds at 257 nm excitation. Spectra were offset for clarity.