

Supporting Information for

Linking Structure to Performance of

$\text{Li}_{1.2}\text{Mn}_{0.54}\text{Ni}_{0.13}\text{Co}_{0.13}\text{O}_2$ (Li and Mn rich

NMC) Cathode Materials Synthesized by

Different Methods

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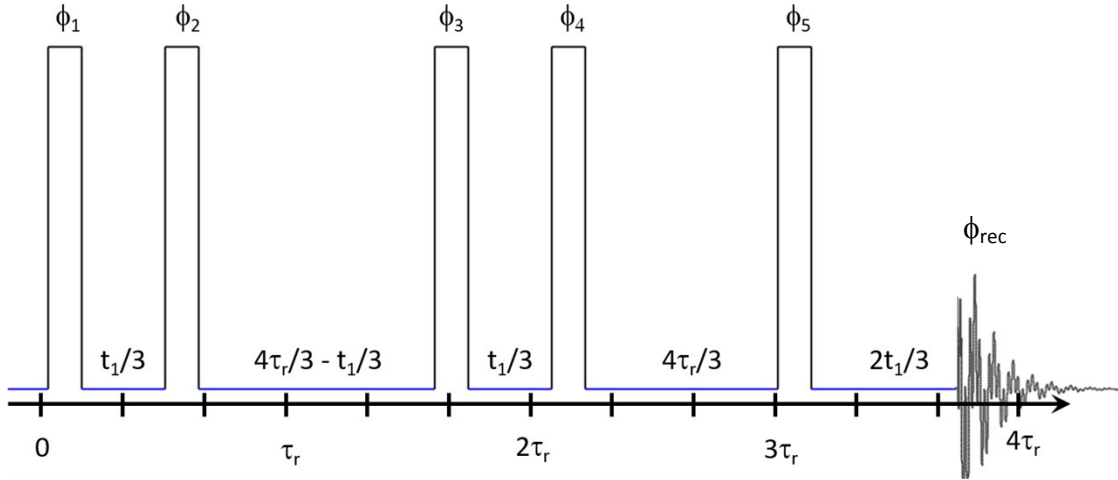


Figure S1: The projection-MATPASS pulse scheme comprising a set of five 90° pulses with irradiation-free periods that generate evolution of the spins in t_1 under a pseudo-infinite spinning speed Hamiltonian thus averaging out any anisotropic interaction. Using a shifted- t_2 acquisition, the magic-angle turning (MAT) portion of the sequence (in the t_1 evolution) is encoded as a phase shift of the FID, thus transforming it into a phase-adjusted sideband separation (PASS) scheme. The result is separation in t_1 according to the order of the sideband and evolution in t_2 according to the anisotropic interactions that under proper shear transformation can be used to correlate isotropic interactions only along one axis with anisotropic interactions only along a perpendicular axis. The rotation period is, τ_r , and the phases of the 5 pulses and the receiver are $\phi_1 = 0$, $\phi_2 = 12n \cdot (2\pi/20)$, $\phi_3 = 10n \cdot (2\pi/20)$, $\phi_4 = 2n \cdot (2\pi/20)$, $\phi_5 = n \cdot (2\pi/20)$, and $\phi_{rec} = 5n \cdot (2\pi/20)$ with $n = 0, 1, 2, \dots, 19$. (see ref 26 in main text for further details about the pulse experiment)

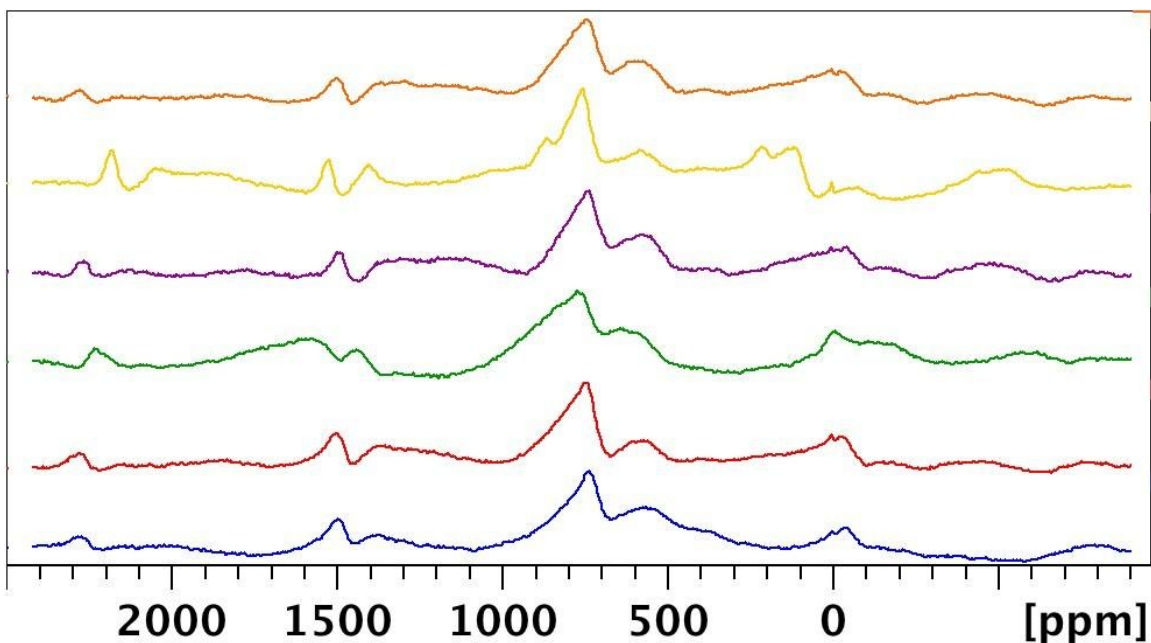


Figure S2: 1D ${}^6\text{Li}$ rotor-synchronized Hahn echo NMR spectra of the LMR-NMC cathode materials prepared, recorded at spinning rates of 30-35 kHz. From the bottom, spectra of the materials from syntheses routes: SS (blue), SG (red), SCR (green), FDno (purple), FDSuc (yellow), FDcit (orange), are shown.

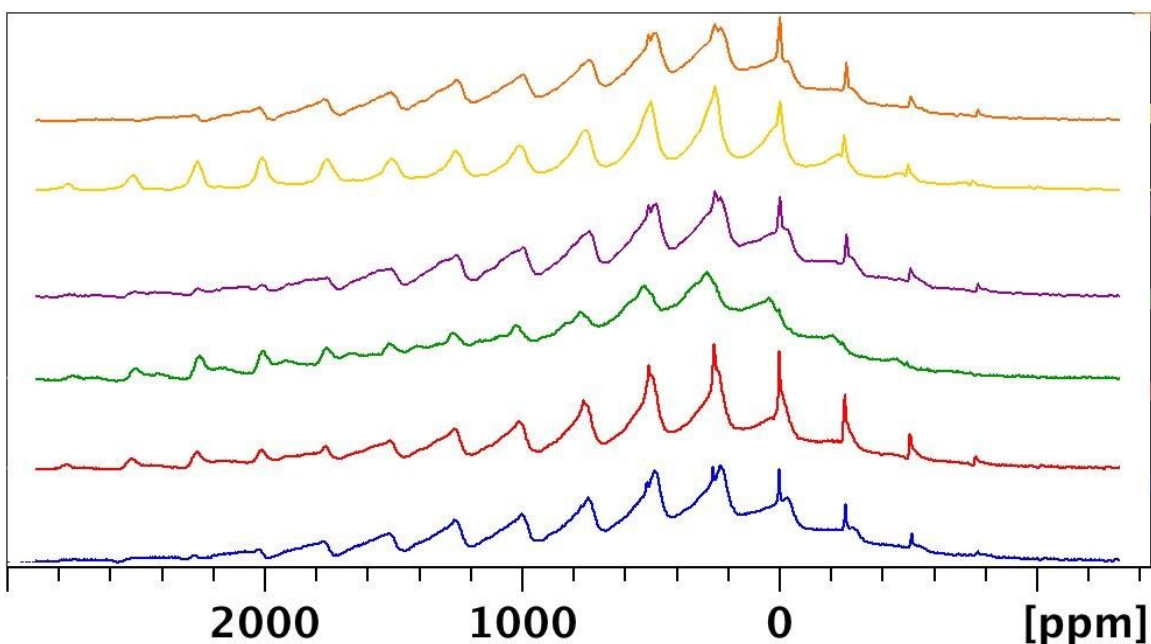


Figure S3: 1D ${}^7\text{Li}$ rotor-synchronized Hahn echo NMR spectra of the LMR-NMC materials prepared, collected at 30 kHz spinning rate. Spectra shown from the bottom are of materials prepared by SS (blue), SG (red), SCR (green), FDno (purple), FDSuc (yellow) and FDcit (orange) synthetic routes.

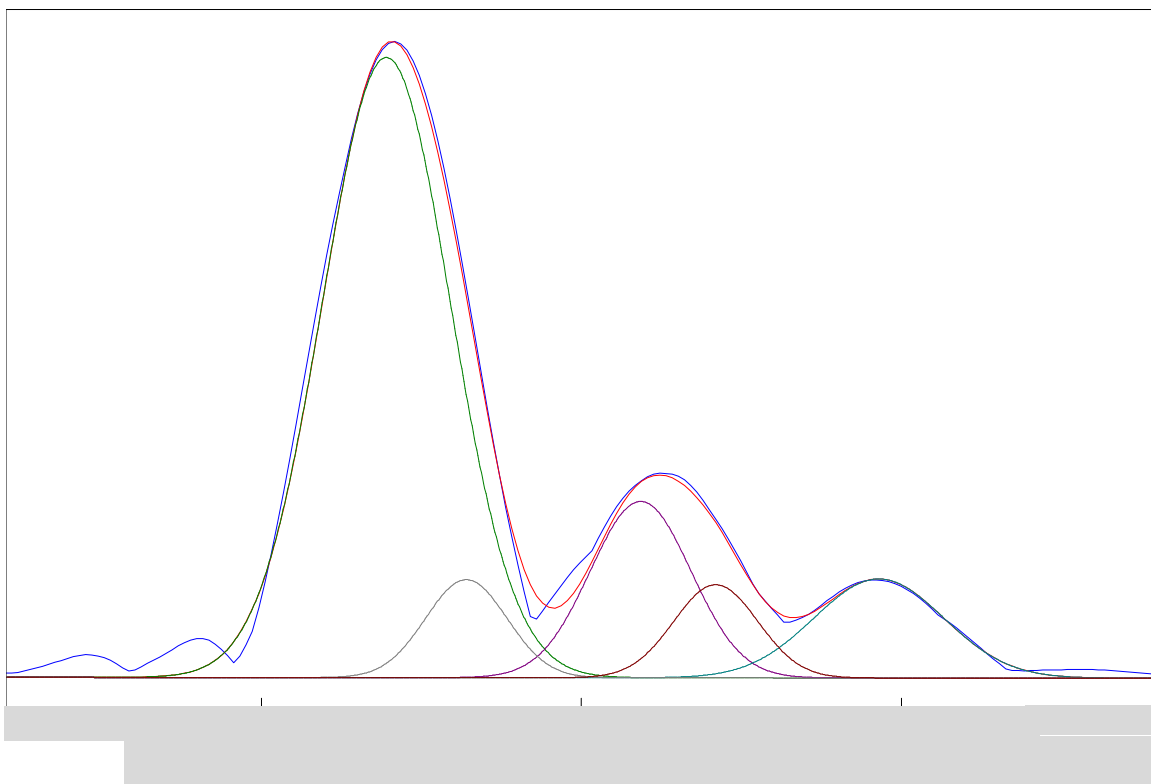


Figure S4: Exemplary deconvolution using the DMFIT program (ref 48 in main text) of the F2 projection from the tilted 2D pjMATPASS spectrum of the FDno material. The simulated spectrum (red) is comprised of lines at 70 ppm (cyan), 580 ppm (brown), 810 ppm (purple), 1360 ppm (grey) and 1600 ppm (green) which fits the experimental spectrum (blue).