Abstract Submitted
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Bond pathway analysis of NMR spectra for $\mathbf{Li_{1.2}Mn_{0.4}Co_{0.4}O_2}$: pristine material HAKIM IDDIR, BARIS KEY, FULYA DOGAN, JOHN RUSSELL, BRANDON LONG, JAVIER BARENO, JASON CROY, ROY BENEDEK, Argonne National Laboratory — NMR has been applied extensively to lithium ion battery cathode materials, of which layered-layered composites $x\mathrm{Li_2MnO_3} \cdot (1 - x)\mathrm{Li}M\mathrm{O_2}(M = \mathrm{Mn,Co,Ni})$ are of particular interest, owing to their high energy density. In this work, NMR spectra are measured for the model layered-layered system $x\mathrm{Li_2MnO_3} \cdot (1-x)\mathrm{LiCoO_2}$ and Bond-Pathway-model analysis is applied to elucidate the atomic arrangement and domain structure of this material (in its pristine state, before electrochemical cycling). The simplest structural element of a domain consists of a stripe of composition LiMn2 parallel to an in-layer crystallographic axis in a metal layer of the composite. A simple model of the composite structure may be constructed by a superposition of such stripes in an LiCoO background. We show that such a model can account for most of the features of the observed NMR spectra.
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