Nuclear Magnetic Resonance for the Characterization of Battery Materials †

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Abstract:
Nuclear Magnetic Resonance spectroscopy is especially useful for the characterization of the chemical nature of the environments of ^{7}Li spins. In materials like $LiVPO_4F$, the structure seems well ordered, as seen by XRD or TEM, however, ^{7}Li NMR spectroscopy shows that 10-20% of the lithium content is in a different environment than the crystallographic site. Dipolar correlation experiments show that these lithium atoms are within a nanometer of the main site, and therefore are defects within the structure.
On the other hand, pulsed field gradients can also provide the positions of ^{7}Li spins in space. This feature is the key to the success of MRI of working batteries. Moreover, the spectra of the cathodes and anodes in a working battery can be separated in situ by PFG-NMR, and the power of spectroscopic imaging is demonstrated in a $LiCoO_2/Li_4Ti_5O_{12}$ battery. In favourable cases, the lithiation front can be observed in thick electrodes with a 100 μm resolution, highlighting the limitation in lithium transport in electrodes with porosity issues.

Contribution: Invited