**Solid State NMR Studies of A Paramagnetic Material—Li1.2Ni0.13Mn0.54Co0.13O2**

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**Introduction**

The rechargeable battery industry has seen extraordinary growth in recent years. Li1.2Ni0.13Mn0.54Co0.13O2, as one of the high-voltage cathodes for Lithium-Ion batteries candidacy, is most promising to further improve the energy density. However, they suffer from dissolution of Mn/Ni in the electrolyte and structural change from layered structure to spinel leading to severe voltage decay and poor cycle performance. In an attempt to alleviate these problems, we are trying to modify the interphase between active material and electrolyte with ZrO2, anatase-TiO2, and rutile-TiO2 coating layers, and investigate the effects of surface modification using advanced solid-state NMR techniques for paramagnetic systems.

**Experimental**

7Li NMR spectra were acquired on a Bruker DRX-300 spectrometer at a Larmor frequency of 116.59 MHz using a Bruker 4-mm MAS probe spinning at 10 kHz. Stimulated pulse sequence and 2D-projection MATPASS pulse sequence were employed for all experiments with different conditions.

**Results and Discussion**

From the 7Li NMR spectra, the 2D-projection MATPASS pulse sequence offers higher resolution than the stimulated pulse sequence and resolved different lithium environments. In future studies, cycled cathode materials will be characterized using 2D projection-MATPASS to evaluate the effects of different types of surface coating.

**Conclusions**

The 2D-projection MATPASS NMR has significantly improved the spectral resolution of paramagnetic battery materials and is useful for distinguishing various Li local environments, which is necessary to investigate paramagnetic battery systems.

**Acknowledgements**

A portion of this work was performed at the National High Magnetic Field Laboratory, which is supported by National Science Foundation Cooperative Agreement No. DMR-1157490 and the State of Florida. Additional support for this project was provided by start-up funds to Y.Y. Hu.

**References**

[1] Hung, I., *et al*., J. Am. Chem. Soc., **134**, 1898-1901 (2012).



**Fig 1.** 7Li NMR spectrum on Li-rich material by

by using stimulated pulse sequence

**Fig 2.** 7Li NMR spectrum on Li-rich material by

by using 2D-projection MATPASS pulse sequence