Developing and applying new tools to understand how materials for Li and "beyond-Li" battery technologies function

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Rechargeable batteries have been an integral part of the portable electronics revolution and are now playing an increasingly important role in transport and grid applications, but the introduction of these devices comes with different sets of challenges. New technologies are being investigated, such as those involving using sodium and magnesium ions instead of lithium, or involving the flow of materials in an out of the electrochemical cell (in redox flow batteries). Importantly, fundamental science is key to producing non-incremental advances and to develop new strategies for energy storage and conversion.

This talk will describe starting with NMR studies of local structure and dynamics. In particular, the analysis of hyperfine interactions between the Li nuclei and paramagnetic ions will be described, focusing on the cathode material NMC-811 ($Li[Ni_{0.8}Co_{0.1}Mn_{0.1}]O_2$). Via an analysis of the hyperfine shifts, information can be obtained concerning the electronic structures of the materials as a function of state of charge, which can be used to understand how these materials function. Li NMR spectroscopy can also be used to quantify dynamics in these materials as a function of vacancy concentration and structural changes. We shall show how these dynamics then affect the mechanisms by which Li are removed from and reinserted into the structure. This work involves the use of new optical methods to study phase transitions at the particle level *operando*, i.e., while the batteries are being cycled. Finally, new results on extremely high-rate batteries will be outlined, making use of a variety of techniques including *operando* NMR spectroscopy.