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Multinuclear Solid State NMR Studies of Lithium Battery Materials

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2:15 p.m.

101 Goergen Hall

Fundamental materials research is essential to move present-day energy storage technologies to the scale needed to develop all-electric vehicles and to manage intermittent sources such as wind and solar. Comparable advances are also required to develop compact power sources for new medical and military/aerospace applications. Structural studies of materials utilized in lithium battery technology are often hampered by the lack of long-range order found only in well-defined crystalline phases. Powder x-ray diffraction yields only structural parameters that have been averaged over hundreds of lattice sites, and is unable to provide structural information about amorphous compounds. Our laboratory utilizes both liquid and solid state nuclear magnetic resonance (NMR) methods to investigate structural and chemical aspects of lithium ion cathodes, anodes, electrolytes, interfaces and interphases. NMR is element- (nuclear-) specific and sensitive to small variations in the immediate environment of the ions being probed, for example Li^+ , and in most cases is a reliably quantitative spectroscopy in that the integrated intensity of a particular spectral component is directly proportional to the number of nuclei in the corresponding material phase. NMR is also a powerful tool for probing ionic and molecular motion in lithium battery electrolytes with a dynamic range spanning some ten orders of magnitude through spin-lattice relaxation and self-diffusion measurements. A survey of brief summaries of several recent NMR investigations will be presented: (i) single crystal studies of LiMPO_4 ($M = \text{Fe}, \text{Co}, \text{Ni}$) lithium ion battery cathodes; (ii) electrode passivation in lithium ion batteries; (iii) structural aspects of CF_x primary lithium battery cathodes and hybrid CF_x /silver vanadate cathodes for medical devices; (iv) natural abundance ^{17}O studies of Li^+ ion solvation in carbonate-based electrolytes.