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NMR Investigations of Structure and Dynamics in Polymers for Energy Storage Applications[1]

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Materials innovation is needed to realize major progress in energy storage capacity for lithium batteries and capacitors. Polymers hold considerable promise as ion conducting media in batteries and electrochemical capacitors and as dielectrics in thin film capacitors. Structural studies of materials utilized in lithium battery technology are hampered by the lack of long-range order found in well-defined crystalline phases. Powder x-ray diffraction yields structural parameters that have been averaged over hundreds of lattice sites, and is unable to provide structural information about amorphous phases. Our laboratory uses 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. Broadband relaxometry based on Fast Field Cycling NMR (FFCNMR) methods can span three to four of these orders of magnitude in a single set of measurements. Results of several recent NMR investigations performed on our lab will be presented. We explore the ion transport mechanism in polyether-based and lithium polymer electrolytes and those based on other base polymers, in particular, the extent to which ionic motion is coupled to polymer segmental motion. Polycarbonates are being considered as a possible replacement for polypropylene in high power thin film capacitors due to their favorable dielectric properties. We investigate the effects of incorporation of two types of additives in the polymer film on the ring-flip motions corresponding to the γ relaxation: (i) high dielectric constant ceramic particles; (ii) polar organic diluent molecules, The low frequency realm of broadband relaxometry allows meaningful comparison with dielectric relaxation studies of these samples performed by collaborators.

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