INSIGHT FROM NMR ON THE LOCAL STRUCTURE, ELECTRONIC STRUCTURE AND DYNAMICS IN BATTERY MATERIALS

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Nuclear Magnetic Resonance (NMR) spectroscopy is a powerful tool for investigating the local structure, electronic environment, and dynamics in battery materials. It provides element-specific and site-selective insights into crystalline and amorphous phases, enabling the characterization of ion coordination, phase transitions, and electronic properties.
The study of paramagnetic positive electrode materials presents challenges due to hyperfine interactions that broaden and shift NMR signals. Advanced NMR techniques and DFT modeling are essential to overcome these difficulties and extract meaningful information on lithium environments, redox states, and structural evolution.
For solid electrolytes, NMR provides key insights into ionic dynamics, with relaxation measurements and exchange spectroscopy (EXSY) allowing the quantification of lithium mobility. At electrode-electrolyte interfaces, the use of both ^{6}Li and ^{7}Li nuclei as probes enables the study of lithium transport and interfacial stability.
For negative electrodes, NMR plays a crucial role in understanding lithium intercalation in graphite anodes and monitoring Li plating/stripping phenomena, which are critical for dendrite formation and battery lifespan.
Through selected examples, this presentation will illustrate the unique contributions of NMR in advancing the understanding of battery materials and guiding the development of next-generation energy storage systems.