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Investigation of Li ion battery materials by NMR

Nuclear Magnetic Resonance (NMR) is a powerful local probe technique for investigating the properties of Li ion battery materials. Besides the investigation of local structural properties which may change due to insertion of Li ions, it can be used to gain information on the dynamical processes that occur during charging/discharging of a Li ion battery. In this talk, we will demonstrate the utility of NMR by introducing our results on two different materials, the potential cathode material $LiMnPO_4$, and the anode material SiCN [1,2]. In $LiMnPO_4$, the large magnetic moment prevents the investigation of the dynamical properties. Nevertheless, we will show that there is disorder in the Mn sublattice by comparing the NMR spectra of two different nuclei, ^7Li and ^{31}P. The disorder leads to the relatively poor electrochemical properties of this material, and our results are perfectly consistent with a recent theoretical study which found a formation of a vacancy-polaron complex owing to lattice distortion. In SiCN, we could successfully determine the activation energy E_A and the correlation time t_0 of the Li ion hopping process from temperature dependent ^7Li linewidth and spin lattice relaxation rate, T_1^{-1}, measurements. The frequency dependence of T_1^{-1} indicates that the Li motion on the ms timescale is governed by continuum diffusion rather than jump diffusion. From the NMR spectra, we find evidence that the carbon phases are the major electrochemically active sites for Li storage.

[1] C. Rudisch et al. Phys. Rev. B 88, 054303 (2013)
[2] S.-H. Baek et al. Journal of Power Sources 253, 342 (2014)

Der Vortrag findet um **10:00 Uhr** im Gebäude der Materialwissenschaften, Lichtwiese, Alarich-Weiss-Str. 2, **Raum 77** statt