# Solid-State NMR Studies on $Li^+$ Ion Dynamics and Structure of $Li_{1+x}Al_xTi_{2-x}(PO_4)_3$

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Solid-state nuclear magnetic resonance (NMR) studies of $Li^+$ ion dynamics based on spin-lattice relaxation (SLR) experiments on lithium aluminum titanium phosphates (LATP) are reported. The samples were synthesized by conventional solid-state reaction using stoichiometric amounts of $Li_2CO_3$, $TiO_2$, $(NH_4)H_2PO_4$ and $Al_2O_3$ at high pressure and heated in a Pt crucible up to 1000 °C for 12 hours [1-4]. LATP with different lithium contents is studied with $^7$Li SLR measurements (in the laboratory frame ($T_1$) and rotating frame ($T_{1\rho}$)) as well as multinuclear magic-angle spinning (MAS) NMR experiments. The solid-state SLR experiments were done with a Bruker 600 AV-III spectrometer at a $^7$Li Larmor frequency of 233 MHz over a wide range of temperature. The high-temperature range was achieved using LASER-heating in a 7mm MAS probe at 3 kHz spinning. $^7$Li, $^{27}$Al and $^{31}$P MAS NMR measurements were done using a 4mm MAS probe at 7-11 kHz spinning frequencies.

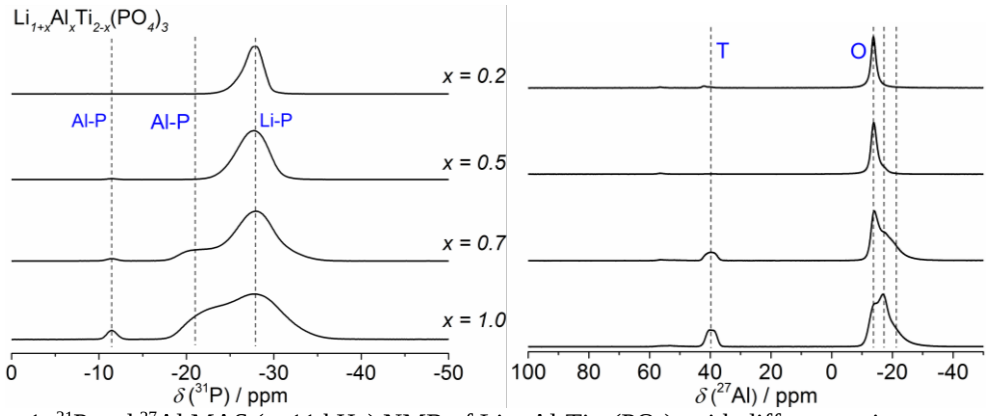


Fig. 1: $^{31}$P and $^{27}$Al MAS (at 11 kHz) NMR of $Li_{1+x}Al_xTi_{2-x}(PO_4)_3$ with different cation contents.

From the diffusion induced $^7$Li NMR SLR rates Li jump rates and activation energies were deduced and the LATPs were found to be fairly fast ion conductors. The different compositions provided signature NMR signals for different cation stoichiometries (Fig. 1). From the various NMR methods, a detailed characterization of LATPs is obtained, with information on local ion dynamics and many structural aspects.

## References

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