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Li-diffusion pathway in the structure of Al-substituted LiTi2(PO4)3

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Due to reaching the stability limit for organic solvents in liquid electrolytes the research on Li-ion batteries adopting solid lithium electrolyte (all-solid-state) becomes of increasing relevance. Among various inorganic solid state lithium conductors the NASICON type compounds are the most promising, where Al-substituted LiTi2(PO4)3 - Li1.3Al0.3Ti1.7(PO4)3 possesses one of the highest ionic conductivities (~10-3 S/cm).
Investigation of series of Al-substituted LiTi2(PO4)3 was carried out. Elastic coherent neutron scattering experiments were performed on the powder diffractometer SPODI at the neutron source FRM II and on the D2B diffractometer at the ILL. Powder diffraction data were collected at room temperature and at fixed temperatures in the range of 100-800 °C (with increment of 100 °C) upon heating. Analysis of the Li positions in the structure as well as the estimation of possible Li-diffusion pathways was performed.

Primary author: MONCHAK, Mykhailo

Presenter: MONCHAK, Mykhailo

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