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Li-ion localisation and mobility in selected solid-state electrolytes probed by neutron diffraction

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The search for new concepts and materials for energy related technology has become a demanding branch in materials sciences and one focus has been shifted to Li- and Na-ion batteries for ready storage and use of energy. One bottle-neck is the use of liquid electrolytes, which induce a number of limitations, device failure due to corrosion and dendritic intergrowth between cathode and anode, etc. Thus, suitable (solid state) electrolyte materials are: among others, two different material groups have been identified, the first ones are Li-bearing garnet type LLZOs, a second are the NASICON –type compounds. A great advantage of NASICON –type materials is, that they work both as Li-ion as well as Na-ion conducting compounds. Suitable solids for the use in batteries are characterized by a high mobility of alkaline ions. This induces several challenges in e.g. localizing light elements, which might be an issue at all using conventional techniques. Neutron diffraction (ND) at non-ambient conditions /temperatures) is the experimental method of choice to give a deep insight into light element distribution in the crystal structure, ion-mobility and transport properties in modern energy related materials. In the talk we will report on recent progress obtained using single crystal and powder neutron diffraction of doped LLZO garnet type Li7La3ZrO12, Li-based NASCON type Li1+xTi2-x(Al,Fe)(PO4)3 and anti-perovskite-type Li3-x(OH)xCl materials and highlight the fancy possibilities of ND.

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