## MLZ User Meeting 2021



Contribution ID: 37

Type: Poster

## Na-ion diffusion in NASICON solid electrolyte material studied by Quasi-Elastic Neutron Scattering

Wednesday 8 December 2021 10:30 (1h 30m)

The sodium superionic conductor (NASICON) materials have been a widely studied class of solid electrolytes for Na-ion based all-solid-state batteries due to their high conductivity and facile synthesis conditions. The aim of this work is to elucidate the reason for extremely high conductivity exhibited by some compositions, specifically by  $Na_{1+x}Zr_2Si_xP_{3-x}O_{12}(0 \ge 3)$ . We investigate the role of the monoclinic to rhombohedral phase transition for the material with x=2.4, which occurs at  $\approx 170$ °C, on the Na-ion occupancy in the crystal structure. Additionally, we study the influence of other dopant elements (Sc and Y) on the Na<sup>+</sup> ionic conductivity. Quasielastic neutron scattering (QENS) is used to measure spatial and temporal dynamic properties of diffusion of Na<sup>+</sup> ions in the crystal lattice. The measurements were performed at the BASIS spectrometer at the Spallation Neutron Source, Oak Ridge National Laboratory in Tennessee, USA. For the evaluation of the QENS data, the DAVE software (NIST Center for Neutron Research) is used. Important information about the Na<sup>+</sup> ion diffusion process, such as activation energies, jump distances between the occupation sites and characteristic times of jumps can be extracted from the measured QENS data. The detailed data analysis is still in progress. This worked was performed as a collaboration between TUM (Heinz Maier-Leibnitz Zentrum, FRM II) and Forschungszentrum Jülich (IEK-1) in the frame of the BMBF project ExcellBattMat cluster.

## Author: PIVARNÍKOVÁ, Ivana

**Co-authors:** Dr SEIDLMAYER, Stefan; Dr FINSTERBUSCH, Martin (Forschungszentrum Jülich GmbH); Mr DÜCK, Geralt (Forschungszentrum Jülich GmbH); Dr NAQASH, Sahir (Forschungszentrum Jülich GmbH); Dr JALARVO, Niina (Neutron Scattering Division, Oak Ridge National Laboratory); Prof. MÜLLER-BUSCHBAUM, Peter (TU München, Physik-Department, LS Funktionelle Materialien); Dr GILLES, Ralph

Presenter: PIVARNÍKOVÁ, Ivana

Session Classification: Poster Session II

Track Classification: Material Science