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

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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 $Na_{1+x}Zr_2Si_xP_{3-x}O_{12}(0\ \mathrm{x}\ 3)$. We investigate the role of the monoclinic to rhombohedral phase transition for the material with x=2.4, which occurs at ≈170℃, on the Na-ion occupancy in the crystal structure. Additionally, we study the influence of other dopant elements (Sc and Y) on the Na^+ ionic conductivity. Quasi-elastic neutron scattering (QENS) is used to measure spatial and temporal dynamic properties of diffusion of Na^+ 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^+ 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.

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