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Time- and space information of proton dynamics in hydrogen bond networks in Fe2+Fe3+3.2(Mn2+,Zn)0.8(PO4)3(OH)4.2(HOH)0.8

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The time and length scales for fast proton dynamics in several ps over hydrogen bonds (HBs) in the title compound could be determined from quasi-elastic neutron scattering (QENS) at TOFTOF. Its dielectric response in a wide frequency range of 1 Hz - 3 GHz from 30 K to 500 K is implicated in its structural properties revealed by Rietveld refinements using neutron powder diffraction data (SPODI). The evolution of three distinct phonons in an energy range of -15 meV and -50 meV from 250 K to 400 K detected in QENS can be addressed to collective motions of the framework polyhedra as OH and HOH groups form their ligands with oxygens. Two distinctly decoupled proton dynamic processes occur in this system: at high temperatures, global protonic transport is thermally activated over an energy barrier (EB) of 0.49 eV. At low temperatures, relaxational proton hopping between double-well potentials in HBs is activated at EB = 0.62 eV. An extremely fast relaxation time in several ps continuously slows down to ~100 s before the entrance into an orientational proton-glass state at about 125 K. Isosurface of bond valence energy landscape maps of H+ at 0.49 eV clearly evidence the honeycomb-shaped route for the protonic conductivity at 393 K, which accords with neutron scattering length densities reconstructed by the Maximum-Entropy Method.

Primary authors: PARK, Sohyun (LMU); Dr LOHSTROH, Wiebke (FRM2); Dr LUNKENHEIMER, Peter (Experimental Physics V Center for Electronic Correlations and Magnetism, University of Augsburg); Dr HOELZEL, Markus (FRM2)

Presenter: PARK, Sohyun (LMU)

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