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Characterization of Phosphide-Based Lithium Ion Conductors by Neutron Powder Diffraction

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In order to attain fast lithium conducting solid electrolytes for the development of high-energy-density all solid state batteries phosphide-based materials have recently gained much interest. With the phosphidotetrelates Li8TtP4 (Tt = Si,Ge) and Li14TtP6 (Tt = Si,Ge,Sn) several lithium conducting materials are already discovered which achieve conductivities up to 1.7mS/cm at RT.[1-4] Recently we extended this material class with the novel superionic conductor Li9AlP4 which has as an undoped material a remarkable fast ionic conductivity of ~3mS/cm at RT and a low activation energy of ~29kJ/mol.[5] Neutron powder diffraction analysis confirms the Li sub-lattice in Li9AlP4 with partial occupied and even lithium split positions. Temperature-dependent measurements reveal the phase transformation from an ordered into a disordered modification which exhibits the same structure type as found in Li14SiP6. Furthermore the crystal structures of the new compound Li8SnP4 was thoroughly analyzed by neutron powder diffraction and other methods. Maximum entropy and one-particle potential evaluations of nuclear density maps give insights into the 3D lithium ion diffusion.

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