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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 Li_8TtP_4 (Tt = Si,Ge) and $\text{Li}_{14}\text{TtP}_6$ (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 Li_9AlP_4 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 Li_9AlP_4 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 $\text{Li}_{14}\text{SiP}_6$. Furthermore the crystal structures of the new compound Li_8SnP_4 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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