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Fast Ionic Conductivity in the Most Lithium-Rich Phosphidosilicate $Li_{14}SiP_6$

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The development of all-solid-state batteries as high power and energy density storage devices has become one of the key challenges in solid-state chemistry and material science. Not only improvement of current electrode and electrolyte materials as well as the cell architecture, but also the search for new compounds is necessary to get access to a new generation of all-solid-state battery technology.
Recently, a new class of promising Li^+ conductors has been studied intensively. Lithium phosphidosilicates and -germanates offer, analogously to oxidosilicates, thiosilicates and thiophosphates, a large structural variety combined with decent Li^+ conductivity up to 10^{-4} S cm^{-1} at 25 °C.
Latest studies report on the preparation and characterization of the most lithium-rich phosphidosilicate $Li_{14}SiP_6$ revealing fast ionic conductivity of $\sigma > 10^{-3}$ S cm^{-1} at 25 °c. Characterization via X-ray diffraction (powder and single crystal) and elastic coherent neutron scattering experiments enabled the thorough investigation of the structural and thermal behavior of the compound. Activation energies, ionic and electronic conductivities have been determined using solid-state ^7Li NMR measurements as well as electrochemical impedance spectroscopy. Finally, diffusion pathways were analyzed by temperature-dependent powder neutron diffraction measurements in combination with MEM and DFT calculations to extend the knowledge about the material properties.

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