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Lithium Diffusion and Ionic Conductivity in Lithium Phosphidotetrelates

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High-performance energy storage solutions are a basic prerequisite for efficient portable devices and the electrification of the transport sector, and by this reaching the CO_2 emission targets. The market and progress demand for advances in electrochemical energy storage and a promising approach towards advanced batteries is the so-called all solid state battery concept, where the liquid electrolyte is replaced by a solid state ion conductor.
In this context, search for new types of lithium-permeating membranes along with detailed investigations of potential solid electrolytes are required. The key target is the understanding of structure-property relationships of solid ion conductors, which is inevitable for a purposeful tailoring of a batch of properties directly relevant for applications.
Material classes such as the family of lithium phosphidotetrelates and -trielates, which contain numerous compounds that combine both a great structural variety and closely related structures, are of particular importance because of their diversity, high lithium conductivity, processability etc.[1−3] Herein, the details of lithium diffusion in a series of structurally related fast ion conducting phosphidotetrelates (e.g., $Li_{14}TtP_6$ and (α-/β-)Li_8TtP_4; Tt = Si, Ge, Sn) are analyzed and compared with respect to the corresponding materials properties. Applying electrochemical impedance spectroscopy and temperature-dependent powder neutron diffraction experiments in combination with the maximum entropy method as well as one-particle potential analysis, enables a thorough study of lithium transport in this class of materials.

[1] S. Strangmüller, et al., *J. Am. Chem. Soc.*, **2019**, *141*, 14200-14209.
[2] T. M. F. Restle, et al., *Angew. Chem., Int. Ed.*, **2020**, *59*, 5665-5674.
[3] S. Strangmüller, et al., *J. Mater. Chem. A*, **2021**, *9*, 15254-15268.

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