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Structural investigation of Li6PS5Cl for applications in all-solid-state batteries

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In the recent years the application of lithium-ion-batteries has attracted a greater interest for large scale applications such as electric vehicles (EV). Liquid batteries are already used and commercialized for such applications. This battery type has higher safety concerns in terms of leakages and flammability, especially in case of a crash. A good alternative with lower risks for drivers and passengers are all-solid-state batteries. Typical materials are polymers, oxides and sulfides. Polymers show a conductivity up to 10-3 S/cm at about 80 ℃, whereas oxides have similar conductivities at room temperature. Sulfidic materials can reach up to 10-2 S/cm which is similar or even better than liquid batteries. One typical crystalline sulfidic material is Li6PS5Cl with an argyrodite like structure. A better understanding of its structure, structural changes and its impact on lithium ion conduction pathways over a large temperature range is necessary. An intensive investigation on Li6PS5Cl with Synchrotron and Neutron diffraction methods will be presented in this work.

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