Poster Presentation

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Superionic phase transitions in anti-fluorite structures

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Fast ion conductors attract continuous and increasing interest in view of possible applications in battery technology. Early examples of superionic phase transitions in anti-fluorite type structures, where the small cations reside in a tetrahedral cage of large anions include Ag2Te [1]. At elevated temperatures anharmonic atom thermal displacements induce cation diffusion towards the large void formed by the central anion octahedron. Of the anti-fluorite structure type compounds Li2 X, where X=(O, S, Se, Te), the compounds Li2O and Li2S showed diffuse transitions to a superionic phase. Very recent advances in battery technology of these compounds [2] motivated us to investigate the end member Li2Te [3] by temperature dependent neutron powder diffraction. The quasi-harmonic temperature dependence of the Li thermal displacement factor shows a distinct steepening of slope around 400°C, indicating a phase transition to a superionic phase. Analysis of derived probability density functions and atom potentials again reveal a corresponding increase of anharmonic, anisotropic Li-ion motion towards the octahedral void. This indicates opening up of Li-ion diffusion pathways at the phase transition. The superionic phase transitions of the Li2X anti-fluorite type structures are steered by their cation-anion distance ratio, which in turn determines their respective transition temperatures. The superionic phase transitions mark the onset of cation sublattice melting, where these transition temperatures are proportional to the melting temperatures of the entire compounds.

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