Structure and Temperature Dependence of Dynamical Properties of Fluoride Crystals

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The fluoride crystals CaF 2 and LaF 3 are superionic conductors with a strong increase of fast ionic conductivity at 1430 K and 1150 K, respectively. We compare the structural and dynamical properties determined with the help of ab initio calculations with results from inelastic neutron scattering experiments. Phonon dispersion curves reflect the structure of a material. We want to investigate the transition to the ionic conductivity by the study of the lattice dynamics. Single crystal (TAS) inelastic neutron scattering studies have been carried out to investigate the temperature dependence of the lattice dynamics of these systems. We observed a strong decrease of a low frequency phonon branch in CaF 2 which is attributed to oscillations in the fluorine sublattice. In contrast, for LaF 3 we have detected a shift to higher frequencies for one dispersionless mode with increasing temperature. The line widths of several modes increase enormously with temperature. In our calculations we consider the temperature dependence regarding the volume dependence of different quantities. Additionally we have obtained indications that the most often published structure of LaF 3 is not stable. Frequencies calculated in the harmonic approximation are compared with experimental data.