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Combined experimental and ab-initio studies of Ca3Ti2O7 local structure

Abstract

Techniques for studying short-range interactions have been successfully used to evaluate local parameters of crystals with high precision. In particular, experiments using perturbed angular correlation (PAC) spectroscopy were able to track the high-temperature phase transitions of hybrid improper ferroelectrics. Here, we continued such works by combining PAC spectroscopy with electronic structure calculations based on the density functional theory to study the evolution of the electric field gradient at the Ca sites of Ca 3Ti2O7. Our results show a structural phase transition from the low-temperature A21am structure to a second phase above 1050 K. This second environment found above the critical temperature is characterized by an electric field gradient distribution with high axial asymmetry. In agreement with the probing of a locally distorted environment, the high-temperature results are compatible with the Acaa structural symmetry. These results contradict previous reports on a direct structural transition from the polar A21am to the aristotype I4/mmm symmetry.

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