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Static and dynamic properties of $PbTiO_3$ at finite temperatures[1]

BRAJESH MANI, INNA PONOMAREVA, Department of Physics, University of South Florida, Tampa, Florida 33620, USA — The ABO_3-type perovskite crystals are key to several important technological applications. To mention a few, electro-optics, waveguides, laser frequency doubling and high capacity computer memory cells. In this work, we develop a route to first-principles parametrization of effective Hamiltonian for ferroelectric ferovskites [1] which allows an accurate description of both static and dynamic properties of such materials. We use this method to examine softening of the transverse optical mode in both paraelectric and ferroelectric phases of $PbTiO_3$. The computed static and dynamic properties are in good agreement with the available theoretical and experimental data. Our study also predicts a crossover between a displacive to an order-disorder transition near the Curie point.

[1] W. Zhong, D. Vanderbilt, and K. M. Rabe, Phys. Rev. B **52**, 6301 (1995).

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