

Abstract Submitted
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Finite-temperature properties of PMN-PT from atomistic simulations¹ ABDULLAH AL-BARAKATY, Umm Al-Qura University, SERGEY PROSANDEEV, LAURENT BELLAICHE, University of Arkansas — Relaxor-based single crystals such as $(\text{PbMg}_{1/3}\text{Nb}_{2/3}\text{O}_3)_{1-x}(\text{PbTiO}_3)_x$ (denoted as PMN-PT) have been reported to exhibit excellent electromechanical properties. The high electromechanical performance characteristics of the relaxor-PT solid solutions is found for compositions at or near the morphotropic phase boundary (MPB) separating the rhombohedral and tetragonal phases. In addition to this MPB area, PMN-PT solid solutions are very interesting and complex to mimic because one of its end-member (PMN) is considered as the prototype of relaxors while its other end-member (PT) is a prototype of classical ferroelectrics. In this work, we developed an effective Hamiltonian technique to theoretically investigate the MPB area of PMN-PT and the symmetries of its phases and to reveal the effect of atomic ordering on physical properties of PMN-PT. If time allows, we will also discuss the effect of oxygen vacancies on the finite-temperature properties of PMN-PT.

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