

Abstract Submitted
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Study of Temperature-Graded Ferroelectrics Using First-Principle-Based Approaches¹ QINGTENG ZHANG, INNA PONOMAREVA, University of South Florida — Temperature-graded ferroelectrics have attracted a lot of attention in the recent years owing to their many remarkable properties. Here we develop a microscopic approach based on first-principles effective Hamiltonian to simulate temperature-graded ferroelectrics. Accuracy of such approach is confirmed by comparing our computational results for $(\text{Ba}_{0.75}\text{Sr}_{0.25})\text{TiO}_3$ alloy with available experimental data. Our computations further reveal: 1) strong anisotropy in polarization response: the polarization offset along the temperature gradient is an order of magnitude smaller than in the perpendicular direction; 2) coexistence of different phases (including low-symmetry phases) in chemically homogeneous regions; 3) rotation of polarization in response to temperature gradient in the unclamped samples. These findings could potentially lead to many novel applications such as energy converters, thermally tunable devices and efficient photovoltaics [1].

[1] Q. Zhang *et al*, Phys. Rev. Lett. **105**, 147602 (2010).

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