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Finite-Temperature Properties of Ba(ZrTi)O3 Relaxors from First Principles[1] SERGEY PROSANDEEV, University of Arkansas, ALI AKBARZADEH, Rice University, ERIC WALTER, College of William and Mary, ABDULLAH AL-BARAKATY, Umm Al-Qura University, LAURENT BELLAICHE, University of Arkansas — A first-principles-based technique is developed to investigate the properties of Ba(ZrTi)O3 relaxor ferroelectrics as a function of temperature. The use of this scheme provides answers to important, unresolved and/or controversial questions such as the following. What do the different critical temperatures usually found in relaxors correspond to? Do polar nanoregions really exist in relaxors? If yes, do they only form inside chemically ordered regions? Is it necessary that antiferroelectricity develop in order for the relaxor behavior to occur? Are random fields and random strains really the mechanisms responsible for relaxor behavior? If not, what are these mechanisms? These ab initio based calculations also lead to deep microscopic insight into relaxors.

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