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Phase diagram of PZT solid solutions near the morphotropic phase boundary from first principles I. KORNEV, L. BELLAICHE, University of Arkansas, Fayetteville, Arkansas 72701, USA, P.-E. JANOLIN , B. DKHIL , Laboratoire Structures, Proprietes et Modelisation des Solides, Ecole Centrale Paris, France, E. SUARD, Institut Laue-Langevin, Grenoble Cedex, France — A first-principles-derived scheme, that incorporates ferroelectric and antiferrodistortive degrees of freedom, is developed to study finite-temperature properties of $Pb(Zr_{1-x}Ti_x)O_3$ solid solutions near its morphotropic phase boundary [1]. The use of this numerical technique (i) resolves controversies about the monoclinic ground-state for some Ti compositions, (ii) leads to the discovery of an overlooked phase, and (iii) yields three multiphase points, that are each associated with four phases. Additional neutron diffraction measurements strongly support some of these predictions. [1] Igor A. Kornev, L. Bellaiche, P.-E. Janolin, B. Dkhil, and E. Suard, *Phys. Rev. Lett.* **97**, 157601 (2006) This work is supported by ONR grants N00014-04-1-0413, N00014-01-1-0600 and N00014-01-1-0365, by NSF grant DMR- 0404335, and by DOE grant DE-FG02-05ER46188.

I. Kornev
University of Arkansas, Fayetteville, Arkansas 72701, USA

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