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Enhanced ferroelectric polarization and potential morphotrophic phase boundary in PZT-based alloys DAVID PARKER, MICHAEL MCGUIRE, Oak Ridge National Laboratory, DAVID SINGH, Dept. of Physics and Astronomy, University of Missouri, Columbia MO — We present a combined theoretical and experimental study of alloys of the high performance piezoelectric PZT ($PbZr_{0.5}Ti_{0.5}O_3$) with BZnT ($BiZn_{0.5}Ti_{0.5}O_3$) and BZnZr ($BiZn_{0.5}Zr_{0.5}O_3$), focussing on lattice instabilities, atomic displacements and ferroelectric polarization. From theory we find that the 75 - 25 PZT - BZnT alloy has substantially larger cation displacements, and hence ferroelectric polarization than the PZT base material, on the tetragonal side of the phase diagram. We also find a possible morphotrophic phase boundary in this system by comparing displacement patterns and optimized c/a ratios. Experiments indicate the feasibility of sample synthesis within this alloy system.

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