

Abstract Submitted
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First-principles calculations of epitaxially strained PbZrO_3 : Coexistence of antiferroelectricity and ferroelectricity SEBASTIAN E. REYES-LILLO, KARIN M. RABE, Department of Physics and Astronomy, Rutgers University — The antiferroelectric (AFE) - ferroelectric (FE) field-induced transition has important applications in energy-storage capacitors and piezoelectric devices. PbZrO_3 is the best known AFE material. Polycrystalline and single crystals PbZrO_3 possess a stable AFE ground state below 505 K. In thin films, experimental results show coexistence of antiferroelectricity and ferroelectricity at room and low temperatures. First-principles calculations of epitaxially strained PbZrO_3 are carried out to give further evidence of this coexistence and to study the polarization switching path. The space groups of the AFE and FE structures are identified together with their important structural and electrical features.

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