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Antiferroelectricity in ZrO_2 and related AXY compounds from first principles SEBASTIAN E. REYES-LILLO, KEVIN F. GARRITY, KARIN M. RABE, Department of Physics and Astronomy, Rutgers University — The field-induced structural transition in antiferroelectrics has important technological applications in energy-storage capacitors and piezoelectric devices. Recently, antiferroelectricity was reported in zirconia (ZrO_2) [1], which is a widely-used material in electronic devices. In this work, we investigate the nature of antiferroelectricity in thin film ZrO_2 and related AXY compounds. For ZrO_2, we use first principles calculations to provide strong evidence that the experimentally reported field-induced ferroelectric phase is an intrinsic property of ZrO_2. Using a Landau type model, we propose a switching mechanism from the nonpolar tetragonal phase to the orthorhombic polar structure, and we show how to access the ferroelectric phase through epitaxial strain. Drawing on these results, we reexamine a wide variety of related AXY compositions as candidates for antiferroelectrics. Physical descriptors that promote optimal functional properties in antiferroelectrics are identified, and results will be presented.

[1] J. Müller *et al.*, Nano. Lett. 12, 4318 (2012).

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