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**Towards an understanding of antiferroelectricity in $PbZrO_3$ from first principles** BRIAN M. ABBETT, School of Applied and Engineering Physics, Cornell University, KARIN M. RABE, Department of Physics and Astronomy, Rutgers University, CRAIG J. FENNIE, School of Applied and Engineering Physics, Cornell University — For decades, $PbZrO_3$ has been referred to as the prototypical antiferroelectric. According to a recent analysis, an essential requirement for antiferroelectricity is that there is a polar phase almost degenerate with the nonpolar ground state. Indeed, as previously reported, first-principles calculations show that the polar $R3c$ structure of $PbZrO_3$ is only 1 meV per formula unit higher in energy than the nonpolar ground state $Pbam$ structure. Here, we explore the question of how these two structures, which seem to be only distantly related, can be so close in energy. Using first-principles methods we investigate the energy landscape of $PbZrO_3$. We introduce a simple structural model that both describes the relevant, low-energy, structural motifs and captures the gross energy landscape relating to both structures. We use this model (and test with direct first-principles calculations) to explore a possible switching path between the non-polar ground state and the metastable polar structure. Our results provide insight into why $PbZrO_3$ is antiferroelectric, which may prove useful in identifying new antiferroelectric materials.

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