

Abstract Submitted
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Absence of Critical Thickness in an Ultrathin Improper Ferroelectric Film¹ NA SAI, The University of Texas at Austin, CRAIG J. FENNIE, Cornell University, ALEXANDER A. DEMKOV, The University of Texas at Austin — We study the ferroelectric stability and surface structural properties of an oxygen-terminated hexagonal YMnO₃ ultra-thin film using density functional theory. Under an open circuit boundary condition, the ferroelectric state with the spontaneous polarization normal to the (0001) surface, is found to be metastable in a single domain state despite the presence of a depolarizing field. We establish a connection between the result and the role of improper ferroelectric transition. Our results imply that improper ferroelectric ultrathin films can have rather unique properties that are distinctive from those of very thin films of ordinary ferroelectrics.

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