

Abstract Submitted
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Ferroelectricity in corundum derivatives¹ MENG YE, DAVID VANDERBILT, Rutgers Univ — The search for new ferroelectric (FE) materials holds promise for broadening our understanding of FE mechanisms and extending the range of application of FE materials. The known FE materials LiNbO_3 can be regarded as derived from the $A_2\text{O}_3$ corundum structure with cation ordering. Here we consider more general binary ($AB\text{O}_3$) and ternary ($A_2BB'\text{O}_6$) corundum derivatives as an extended class of potential FE materials, motivated by the fact that some members of this class have recently been synthesized. There are four structure types for these corundum derivatives, and the number of cation combinations is enormous, but in many cases the energy barriers for polarization reversal may be too large to allow FE behavior. Here we present a first-principles study of the polar structure, coherent FE barrier, and domain-wall switching barrier for a representative set of polar corundum derivatives, allowing us to identify several potentially new FE materials. We also discuss the conditions under which ferroelectricity is compatible with magnetic ordering. Finally, we identify several empirical measures that can provide a rule of thumb for estimating the barrier energies. Our results should assist in the experimental search for new FE materials in the corundum derivative family.

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