Ferroelectric switching path of polar corundum derivatives

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Polar magnets form one of the most promising classes of materials for multiferroics and spintronics. While much attention has focused on ABO_3 perovskites, recent studies have demonstrated that ABO_3 corundum-derived materials also have remarkable polarization and magnetization properties. In 2008, Fennie studied corundum-structure $FeMO_3$ (M = Fe, Mn, Ni) in the $LiNbO_3$-type phase using symmetry analysis and first-principles calculations.[1] He found that these novel materials exhibit large spontaneous polarizations and weak ferromagnetism. Most interestingly, he found that the two order parameters are coupled so that the magnetization can be switched by 180° when the direction of polarization is reversed by an applied electric field. Motivated by this pioneering work, novel ABO_3 and $A_2BB'O_6$ corundum derivatives have been successfully synthesized in high-temperature and high-pressure conditions.[2–5] Even though these noncentrosymmetric structures exhibit a spontaneous electric polarization, it has remained unclear whether the polarization can be switched by an external electric field. In this work, we use first-principles density-functional methods to study the intrinsic switching path and energy barrier for some of the ABO_3 and $A_2BB'O_6$ corundum derivatives that have been synthesized to date. Generalizing from our results, we clarify the general conditions under which FE switching is possible in this class of materials.

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