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Strong coupling of ferroelectricity and magnetism in the hexagonal ferrites

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During the last decade one of the most extensively studied class of multiferroics has been the hexagonal rare-earth manganites $RMnO_3$ where R=Dy-Lu, Y, Sc. These compounds exhibit antiferromagnetic (AFM) order with a Néel temperature $T_N \approx$ 100K. In addition, they are improper ferroelectrics ($T_C > 1200K$) driven a by zone-tripling structural distortion associated with a buckling of the R-planes and a rotation of the oxygen trigonal bipyramids. The improper nature of the transition is responsible for the fascinating, topologically protected trimer-domains. Even though magnetism and ferroelectricity in these materials are not intrinsically coupled, there is a non-trivial interaction between the structural and magnetic domain walls. In contrast to the manganites, the ground state structure of the rare-earth ferrites $RFeO_3$ is the orthorhombic perovskite. Recently, however, thin films of $RFeO_3$ have been epitaxially stabilized in the hexagonal rare-earth manganite structure. This development has triggered several new studies of these hexagonal ferrite systems. Similar to manganites, ferrites exhibit ferroelectricity above room temperature and crystallize in $P6_3cm$ polar structure but conflicting results have been reported as to the origin of ferroelectricity in these materials. Unlike the manganites, recent neutron diffraction measurements suggest a considerably high AFM ordering temperature, T_N =440 K. Additionally there is an indication of a second temperature, $T_{\mathrm{wFM}} \sim 100K$, at which weak ferromagnetism has been observed. In this work my collaborators (Alex Wysocki and Craig J. Fennie) and I address the nature of ferroelectricity and magnetic order in the $RFeO_3$ systems from first-principles. We elucidate the origin of ferroelectricity in the rare-earth ferrites and provide many useful insights into their magnetic behavior, which we will show is fundamentally different than that observed in the manganites. Combining first-principles calculations with a detailed modeling of the magnetic structure we will also show how this difference leads to an interplay between ferroelectricity and magnetism in the ferrites. This strong coupling, absent in the hexagonal manganites, manifests itself in a nontrivial way that may be useful for voltage controlled magnetic functionalities.