First Principles Investigation of Structural and Electronic Properties of Hexagonal Rare-Earth Ferrites, $RFeO_3$ (R = Lu-Tm)

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The multiferroic hexagonal manganites $RMnO_3$ (R=Dy-Lu,Y) belong to a fascinating class of materials that display an unusual, complex interplay between structural, polar and magnetic domains [1, 2]. The electric polarization in these compounds is found to be a by-product of a trimerized (zone-boundary) lattice distortion, arising from the ionic size mismatch between R^{+3} and Mn^{+3} ions [3, 4]. Both theoretical [4] and experimental [5, 6] studies suggest that an immediate transition from the high temperature paraelectric phase ($P6_3/mmc$) to the trimerized polar phase ($P6_3cm$) takes place in these compounds.

The hexagonal ferrites $RFeO_3$ (R=Er-Lu,Y) crystallize in the same polar structure as the manganite counterparts. However, in case of $YbFeO_3$, one of the members of the hexagonal ferrite systems, the $P6_3/mmc$ to $P6_3cm$ transition is reported to be mediated by an intermediate polar phase ($P6_3mc$) [7]. This indicates a different underlying energetics of the ferrite systems compare to the manganite counterparts, which is verified in the present study through first principles density functional calculations.

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