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 byproduct 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$_3$cm) 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$_3$cm transition is reported to be mediated by an intermediate polar phase (P6$_3$mc) [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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