Most of the hexagonal manganite compounds are ferroelectric with a high ferroelectric transition temperature and order magnetically around 100 K. In case of hexagonal ferrites, Fillipetti, Spaldin, and Rabe have reported the hexagonal manganite systems, First principles investigation of structural and electronic properties of hexagonal rare-earth ferrite systems, RFeO₃ (R = Lu - Er), Phys. Rev B, Nature Materials 2004. Origin of Ferroelectricity 

Polarization is a slave to the primary order parameter, ϒ.

\[ F(\Gamma, \Omega) = \frac{1}{2} [a|\Omega|^2 + \frac{1}{4} \beta \Omega^4 - \frac{1}{2} \alpha_\Omega \theta^2 - \frac{1}{4} \beta_\Omega \theta^4] \]

Once primary order parameter becomes non zero, a polarization is induced.

In case of hexagonal manganites the primary order parameter is a zone boundary (Kₗ) phonon mode.

Contribution of zone center polar mode

Effect of epitaxial strain

Conclusions

- From first principles density functional investigation we have shown that similar to hexagonal rare-earth manganite systems hexagonal ferrites are ferroelectric with comparable magnitude of polarization.
- Large polarization is driven by quadratic coupling between Kₗ mode and the polar Γₗ mode.
- Our results indicate a direct transition from the PE P₆₋₃cm to the polar P₆₋₃cm phase.