Engineering 180° magnetoelectric switching phenomena and enhanced magnetization in hexagonal ferrites through carrier doping

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The quest for magnetoelectric (ME) switching mechanisms of controlling magnetic order in systems by the application of electric fields, is an active area of research. Also, engineering multiple quantum phenomena, such as magnetic, ferroelectric and non-trivial topological phenomena, in a single system to enhance its functionalities is at the forefront of the recent research activities. In this regard $LuFeO_3$ type hexagonal oxides hold immense potential as working materials [Nature Communications **5**, 2998 (2014), Nature Materials **13**, 163-167 (2014), Nature **537**, 523-527 (2016), Nature Communications **11**, 5582 (2020)]. $LuFeO_3$ forms an improper ferroelectric order below ~ 1020 K with a robust electric polarization **P** and a canted antiferromagnetic order below 147 K, exhibiting a weak magnetization $|\mathbf{M}|$ ~ 0.03 μ_B/Fe. A cross coupling between **P** and **M** in $LuFeO_3$ type hexagonal systems was proposed by leveraging the cross coupling between non-polar trimer distortions ($\boldsymbol{Q}_{K_3}$) and anti-symmetric exchange interactions between Fe^{+3} ($S = \frac{5}{2}$) magnetic ions [Nature Communications **5**, 2998 (2014)]. In the present study, we report a 180° ME switching mechanism driven by the complex mutual interaction of the multiple magnetic sublattices created within this hexagonal lattice, their evolution and subsequent behavior under the effect of trimer distortions ($\boldsymbol{Q}_{K_3}$). A situation like this can be effected by doping $LuFeO_3$ with carriers. We conceptualized the proposed ME coupling for a doping concentration of $x =$ 1/3 per Fe. The localization of the doped carriers introduces$S = 2$magnetic site within a $S = \frac{5}{2}$ hexagon. Here, we have identified three different magnetic phases and have showed that the transformation of one phase to another strongly depends on the temperature and $\boldsymbol{Q}_{K_3}$. In these magnetic phases the spin orientation of the $S = 2$ sublattice is perpendicular to that of the $S = \frac{5}{2}$ sublattice. This mutually influencing orientation is driven by the Dzyaloshinskii-Moriya (DM) interactions between two sublattices, resulting not only in an enhancement of the net magnetization **M** by order of magnitude, but also in an increase of the magnetic transition temperature compared to the parent system.

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