Origin of room-temperature multiferroism in hexagonal LuFeO$_3$

XIFAN WU, HONGWEI WANG, Physics Department, Temple University, PA 19122, USA, IGOR SOLOVYEV, National Institute for Material Science, Tsukuba, Japan, JIAN SHEN, WENBIN WANG, Department of Physics, Fudan University, Shanghai 200433, China, XIAO WANG, XUEMEI CHENG, Department of Physics, Bryn Mawr College, Bryn Mawr, PA 19010, USA, LIXIN HE, University of Science and Technology of China, Hefei, Anhui, China, XIAOSHAN XU, Department of Physics, University of Nebraska-Lincoln, NE, USA — Combined theoretical and experimental studies are carried out, focusing on the exchange interactions and their couplings with the structural instabilities in hexagonal LuFeO$_3$ (hLFO). We apply an extended Kugel-Khomskii model based on maximally localized Wannier functions generated from band structure calculations. The model clearly shows that the single occupied $d_{z^2}$ orbital in hLFO greatly increases the exchange coupling compared to that of hexagonal LuMnO$_3$ in which $d_{z^2}$ is empty. The interlayer exchange interaction is the key to the spin reorientation (SR) and weak ferromagnetic moment observed below 130K. Our calculations show that SR is strongly coupled to the $K_1$ phonon mode and only weakly dependent on $K_3$ and $\Gamma_2^-$ phonons. It indicates that the atomic displacements along positive direction of $K_1$ mode is responsible for the spin reorientation. This scenario is confirmed by our X-ray diffraction and X-ray absorption experiments. In the end, we propose that $T_{SR}$ can be adjusted to be room temperature by structural competition between $K_1$ and $\Gamma_2^-$ modes in hLFO or by interface engineering.

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