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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, niversity 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 Γ_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 Γ_2^- modes in hLFO or by interface engineering.

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