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First-principles studies of magnetoelectric coupling in hexagonal $LuFeO_3$ under applied electric fields YUBO ZHANG, HONGWEI WANG, PRATIKKUMAR DHUVAD, Temple Univ, XIAOSHAN XU, University of Nebraska, MASSIMILIANO STENGEL, Institut de Cincia de Materials de Barcelona, XIFAN WU, Temple Univ — The recently stabilized hexagonal $LuFeO_3$ thin-film provides an opportunity in realizing the magnetoelectric coupling in multiferroic materials, in which the weak ferromagnetism due to Dzyaloshinskii-Moriya interaction was found to be closely associated with the trimerization (K_3) mode. Here, we performed first-principles calculations in hexagonal $LuFeO_3$ and studied the variations of weak ferromagnetic moment under applied electric fields. It is found that the weak ferromagnetism is a property that can be directly tuned by the external electric fields. As an improper ferroelectric material, such a magnetoelectric coupling is realized by the strong interaction between the trimerization mode and ferroelectric mode. Under the electric field poling, ferroelectric mode will respond. A change in ferroelectric distortion will in turn affect the amplitude of trimerization mode, and therefore, the weak ferromagnetism. Interestingly, the magnetoelectric coupling in $LuFeO_3$ shows a strong nonlinear behavior originating again from the coupling between the trimerization and ferroelectric modes due to its improper nature.

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