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**Energetics of Intrinsic Defects in hexagonal LuFeO<sub>3</sub>**

TULA R. PAUDEL, EVGENY Y. TSYMBAL, Department of Physics and Astronomy Nebraska Center for Materials and Nanoscience, University of Nebraska — The hexagonal Lutetium Ferrite (*h*-LuFeO<sub>3</sub>) is one of the few multiferroic materials where the spontaneous ferroelectric and magnetic ordering are simultaneously present at room temperature. Here, we investigate energetics of the intrinsic defects *h*-LuFeO<sub>3</sub> using the first-principles supercell approach in the dilute limit. We find the possibility of intermixing, i.e., Lu replacing Fe when *h*-LuFeO<sub>3</sub> is grown at the Lu rich conditions, and Fe replacing Lu when this compound is grown at the Fe rich conditions. In addition, our calculations predict the formation of a large number of oxygen vacancies when *h*-LuFeO<sub>3</sub> is grown in the reducing conditions. We find that even when the concentration of oxygen vacancies is large, they do not create as much free charge as they form relatively deep localized defect states. Cation vacancies are predicted to have shallow transition levels and the large formation energy, which makes them unlikely in this compound. The electronic structure of all these defects and their effect on the magnetic and polarization properties of *h*-LuFeO<sub>3</sub> are discussed.

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