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First-principles Investigations of Fe Impurities in $KNbO_3$ MOHUA BHATTACHARYA, STEVEN LEWIS, WILLIAM DENNIS, Department of Physics and Astronomy, The University of Georgia — The perovskite based material $KNbO_3$ has been studied extensively for its photorefractive properties, where the electro-optic effect combined with photoconductivity changes the local refractive index of the material in response to the incident intensities. The presence of a transition metal impurity like Fe is required for efficient photorefractive performance of this material. To shed light on the physical mechanism of this behavior, we perform first-principles calculations within the density functional theory framework. In this talk, we present the geometric and electronic structures of $KNbO_3$:Fe super cells and compare two cases: one in which the Fe^{3+} impurity on the Nb^{5+} site is compensated by an O vacancy in the first coordination shell and one in which the O vacancy is in the second coordination shell. Connections of this work to recent experimental measurements are discussed.

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