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First-principles study of the photorefractive material $KNbO_3$ MOHUA BHATTACHARYA, STEVEN P. LEWIS, WILLIAM M. DENNIS, Department of Physics and Astronomy, University of Georgia, GARY COOK, DEAN R. EVANS, Air Force Research Laboratory — 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. Recent experiments suggest that Ag co-doping enhances the photorefractive properties significantly. To shed light on the physical mechanism of this behavior, we perform first-principles calculations within the density functional theory framework. In this poster, we present the structural relaxation results for the different crystal forms that the pure host $KNbO_3$ can exist in at room temperature and higher. Preliminary calculations about the role of Fe on the geometric and electronic structures of $KNbO_3$ will also be presented.

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