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**Polarization effects in silver delafossite systems** GIHAN PANAPITIYA, JAMES P. LEWIS, West Virginia Univ — Delafossites are a promising class of materials which has applications in catalysis and optoelectronic devices. Even though much work has been carried out on the cuprate family of delafossites, little is known about the structural and electronic properties of it's silver counterpart. In this work, we present a computational study for two delafossite oxides of the form $AgB_{1-x}Fe_xO_2$(For B = Al,Ga). A large number of structures are studied by varying the Fe alloying percentage(x) from 0 to 5 and by choosing the impurity sites randomly. We find that the local structural changes occurring at the vicinity of Fe atoms in these two systems have opposite trends with regard to the O-O distance. The reason for this difference in the trends is identified as the polarization effects on the inter-atomic distances caused by the displacements in O atoms resulting from the incorporation of Fe in sites, previously occupied by either Al or Ga. We believe that these effects are mediated by the differences in the atomic radii of Fe, Al and Ga. Higher alloying levels coupled with nearest neighbor Fe atoms can intensify these distortions in the structure creating deformations in the O-Ag-O bonds, which are directly related to the formation of the conduction band edge in these systems.

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