Abstract Submitted
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Exploration of Ti-doped $CuGaO_2$ delafossite[1] M. KYLEE RICE, JAMES P. LEWIS, West Virginia University — In their most simple form, delafossite materials are of the form ABO_2 where A is a +1 metal cation and B is a +3 metal cation. Since O is in the -2 ionization state in the crystal, this results in a charge balanced and stable crystal. Delafossite materials have been studied for their p-type and n-type conductivity, however. This means that studied material samples have extra holes or electrons due to defects resulting in a net charge and thus allow for conductivity within the sample. Since types of defects inherent in a sample are due to the structure of the sample, they can then be doped with other elements to increase the p- or n-type conductivity. For example, $CuCrO_2$ is found to be of p-type defect chemistry, and when doped with Mg (+2), has a conductivity of 220 S cm^{-1}. In this research we computationally explore electronic properties of a new material, p-type $CuGaO_2$ doped with Ti (+2), and the resulting defects. This delafossite is a wide band gap semiconductor and has shown promise as a p-type material and a photocatalyst with the ability to reduce CO_2 to CO. An understanding of the doping of Ti in $CuGaO_2$ could lead to a material with a smaller band gap, better photocatalytic abilities, and enhanced conduction.

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