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Electronic properties of silver delafossite materials ($AgB_{1-x}Fe_xO_2$) using high-throughput calculations GIHAN PANAPITIYA, JAMES LEWIS, Department of Physics and Astronomy, West Virginia University — Delafossites are promising materials which can be used as photovoltaics or photocatalysts to reduce the CO_2 to viable products such as CH_4 and CH_3OH. In this work, we present a high-throughput computational study for three delafossite oxides of the form $AgB_{1-x}Fe_xO_2$ (For B = Al,Ga,In), in search of candidate materials which can harness visible light. We explore the effect on optoelectronic properties of these materials when the B site is alloyed with Fe. A large number of structures are studied by varying the Fe doping percentage(x) from 0 to 0.05 and by choosing the impurity sites randomly. Statistical analysis is carried out to study the relative positions of the substituent atoms (Fe). We will discuss the structural trends and the optoelectronic properties of these materials to determine their viability in potential photelectrochemical or photovoltaic applications.

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