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The effects of alloying $CuAlO_2$, $CuGaO_2$, and $CuInO_2$ with Fe at low percentage levels RAMON BEESLEY, GIHAN PANAPITIYA, JAMES LEWIS, West Virginia University — Delafossite oxides are a family of materials with the form ABO_2 , where the A-site is a monovalent cation (Cu, Ag, Au) and the B-site is a trivalent cation (Ga, Al, In). Within this family of material both p-type and n-type characteristics can be found. Delafossites typically have a wide optical band gap, this band gap may be tuned by adding a second B-site element forming an $AB_{(1-x)}^1B_{(x)}^2O_2$ alloy. The addition of the second B-site atom changes the electronic structure and may also enhance optical absorption. We studied the effects of alloying $CuAlO_2$, $CuGaO_2$, and $CuInO_2$ with Fe at 0%, 1%, and 2% alloying levels. Using the FIREBALL program we optimized the atomic structure, calculated the total and partial density of states, calculated the valence band edge for each alloy level, and investigated the clustering factor of the second B-site atom in the 2% alloys. From the partial density of state, we looked at each type of atoms contribution to the change in the valence band edge and found that Fe is the major contributor to the change.

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