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Change In The Electronic Structure And Optical Absorption Of Cuprate Delafossites Via B-site Alloying RAMON BEESLEY, GIHAN PANAPITIYA, JAMES LEWIS, West Virginia University, LEWIS GROUP TEAM — 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). 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. We investigate changes in the electronic structure of $CuAlO_2$, $CuGaO_2$, and $CuInO_2$ when alloyed with $CuFeO_2$. Using the FIREBALL program to optimize the atomic structure, calculate the total and partial density of states, calculate the valence band edge for each alloy level, and investigate the clustering factor of the second B-site atom, it is found that alloying with Fe creates midgap states caused by $Fe - O$ interactions. From the partial density of state, each type of atoms contribution to the change in the valence band edge can be seen. Observed changes to the materials include increased optical absorption in the visible range, and symmetry breaking because of the deformation in the crystal structure. The $CuFeO_2$ alloying percentages range from 0-5%. We are synthesizing these alloys to experimentally verify the changes in the optical absorption spectra.

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