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Strain Induced Photoabsorption of $CuGa_{1-x}Fe_xO_2$ M. KYLEE UNDERWOOD, BARRY HAYCOCK, JAMES LEWIS, West Virginia University, JONATHAN LEKSE, CHRISTOPHER MATRANGA, DOE NETL Pittsburgh — Delafossite oxides are a family of materials that hold promise for photocatalytic, thermoelectric, and other cutting edge applications. These materials are of interest because they exhibit a disparity between their optical and electronic band gaps due to inversion symmetry according to the Laporte selection rule. Though they appear transparent, their electronic structure suggests that they should absorb visible light, aside from conduction and valence band parity. We use B-site substitution to break inversion symmetry and allow the absorption of visible light. Here we present computational and experimental electronic and optical results of B-site substitution of the delafossite $CuGaO_2$ with Fe which supports the inversion symmetry theory of the band gap disparity. Included are experimental and computational absorption spectra for $CuGa_{1-x}Fe_xO_2$. We find and explain an interesting increase optical absorption in the visible range at the 5% Fe substitution level. To the best of our knowledge computational results to this degree of percentage accurate substitution or alloying have not been performed on this or similarly complicated systems.

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