Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

High-Throughput Investigation of Delafossite materials[1] BARRY HAYCOCK, M. KYLEE UNDERWOOD, Department of Physics, West Virginia University, WV26506, United States, JONATHAN LEKSE, CHRISTOPHER MATRANGA, The National Energy Technology Laboratory, Pittsburgh, PA 15236, United States, JAMES P. LEWIS, Department of Physics, West Virginia University, WV26506, United States — We present the application of high-throughput calculations to the intriguing problem of the forbidden optical transition in the $CuGa_{1-x}Fe_xO_2$ delafossites, which is prototypical of many delafossite systems. When 5% or more of the Ga sites are replaced with Fe, there is a sudden shift to an optical band gap of 1.5eV from 2.5eV. Using high-throughput calculations and data mining techniques, we show the most likely positional configurations for x = 0.00 through x = 0.10 of the Fe atoms relative to one another. Implications of this result and applications of the techniques used are discussed, including the development of candidate materials via high-throughput analysis of constituent search-space.

[1]Funded by the National Science Foundation through NSF DMR 09-03225 and a subcontract from NETL (URS RES) for Work Activity 0004000.6.600.007.002.420.000.005 ARRA ICMI Project.

Barry Haycock
Dept of Physics, West Virginia University, WV26506, United States

Date submitted: 12 Nov 2012 Electronic form version 1.4