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High Pressure Synthesis of Rhombohedral Delafossite Structured α-$AgGaO_2$ MEYSAM AKHTAR, Department of Physics, University of Louisville, MADHU MENON, Center for Computational Sciences, University of Kentucky, MAHENDRA SUNKARA, Conn Center for Renewable Energy Research, University of Louisville, GAMINI SUMANASEKERA, Department of Physics, University of Louisville, ANDRIY DURYGIN, Center for the Study of Matter at Extreme Conditions, Florida International University, JACEK JASINSKI, Conn Center for Renewable Energy Research, University of Louisville — In this work, we demonstrate for the first time the high pressure synthesis of α-$AgGaO_2$ via a solid state reaction of Ag_2O and Ga_2O_3. Synthesis experiments were carried out at pressures and temperatures up to 10 GPa and 600 C, respectively, using a resistively-heated diamond anvil cell. Electron diffraction confirmed the rhombohedral delafossite crystal structure of the synthesized $AgGaO_2$ and its corresponding lattice parameters of a = 2.99 Å and c = 18.43 Å. The vibrational modes analysis was also conducted using a combination of ab initio density functional theory (DFT) and Raman spectroscopy. This analysis yielded good agreement between the calculated Raman-active modes and experimental Raman data. Finally, the application of the GGA + U formalism-based on DFT to calculate the electronic band structure of α-$AgGaO_2$ provided a more realistic theoretical band gap value than those reported previously.

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