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Ab initio study of structural and electronic properties of $CuAlO_2$ and $AgAlO_2$. JAMES SHOOK, LUISA SCOLFARO, Texas State University — Transparent conducting oxides are an active area of research due to their applications in transparent electronics such as photovoltaic cells and flat panel displays. Of particular interest are $XAlO_2$ (X = Cu, Ag), two p-type oxides with band gaps in the optical range (> 3.0 eV). These oxides are known to exist in three phases: two delafossite structures whose phase depends on stacking order (2H, 3R) and an orthorhombic crystal structure. How each phase compares to one another energetically is still not well understood. To that end, an ab initio study − using Density Functional Theory based calculations with Generalized Gradient Approximation (GGA), GGA+U, with U being the Hubbard atomic potential for the d-orbital, and modified Becke-Johnson approximation for correlation and exchange potentials − on the structural and electronic properties of $XAlO_2$ are presented. The 2H phase is modeled using an 8-atom hexagonal primitive cell while both a 4-atom rhombohedral primitive cell and 12-atom hexagonal unit cell are used to study the 3R phase. The orthorhombic phase is modeled using a 16-atom unit cell. The obtained band structures and density of states results are compared with those in literature and predictions about structural energies for each phase are presented.

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