Electronic and optical properties of the CuAlO$_2$ and AgAlO$_2$ transparent conductor oxides: a first principles study

JAMES SHOOK, LUISA SCOLFARO, Texas State Univ-San Marcos — Transparent semiconductors are an exciting area of research due to their applicability in photovoltaic cells and flat panel displays. Many well-known n-type transparent conducting oxides (TCOs) have been documented, but the search for commercially viable p-type TCOs continues due to characteristically large hole effective masses and low hole mobility arising from the localized valence p-states of O. The delafossites, CuAlO$_2$ and AgAlO$_2$ (XAO), show promise as viable p-type TCOs because of the delocalization of valence states that results from hybridization of Cu/Ag d-states with O p-states. This work presents the electronic and optical properties of 2H-XAO using density functional theory as implemented in the VASP code. The exchange-correlation energy of the 8 atom 2H-XAO hexagonal primitive cell is treated using the generalized gradient approximation and the modified Becke-Johnson approximation with the use of a Hubbard energy correction for the Cu/Ag d-orbitals, in order to obtain values for the band gaps similar to experimental values. Optical properties are derived from the complex dielectric function, which is calculated using the charge density obtained from the self-consistent calculation. The presented work is scrutinized against available experimental results.