X-ray photoelectron spectrum, X-ray diffraction data, and electronic structure of chalcogenide quaternary sulfide Ag2In 2GeS6: Experiment and theory

Abstract

We report measurements of the X-ray diffraction and X-ray photoelectron spectrum on single crystals of $Ag_2In_2GeS_6$. We also present first principles calculations of the band structure and density of states using the state-of-the-art full potential augmented plane wave method with different possible approximation for the exchange correlation potential. In this paper, we make a detailed comparison of the density of states deduced from the X-ray photoelectron spectra with our calculations. The theoretical results of the density of states are in reasonable agreement with the X-ray photoelectron spectroscopy (VB-XPS) measurements with respect to peak positions. The calculated density of states shows there is a strong hybridization between the states in the valence and conduction bands states. We have calculated the electron charge density distribution in the (100) and (110) planes. In the plane (100), there exists Ag, In, and S atoms, while the plane (110) Ag, S, and Ge atoms are present. The bonding properties are obtained from the charge density distributions. The calculation show that there is partial ionic and strong covalent bonding between Ag-S, In-S, and Ge-S atoms depending on Pauling electro-negativity difference of S (2.58), Ge (2.01), Ag (1.93), and In (31.78) atoms.