Materials Research Bulletin, vol.48(11), 2013, pages 4555-4564

Density of electronic states and dispersion of optical functions of defect chalcopyrite $CdGa_2X_4$ (X = S, Se): DFT study

Abstract

A density functional theory (DFT) based on full potential linear augmented plane wave (FPLAPW) was used for calculating the electronic structure, charge density and optical properties of $CdGa_2X_4$ (X = S, Se) compounds. Local density approximation (LDA), generalized gradient approximation (GGA), Engle Vasko generalized gradient approximation (EVGGA) and recently modified Becke-Johnson (mBJ) were applied to calculate the band structure, total and partial density of states. The investigation of band structures and density of states of $CdGa_2X_4$ (X = S, Se) elucidate that mBJ potential show close agreement to the experimental results. The mBJ potential was selected for further explanation of optical properties of $CdGa_2X_4$ (X = S, Se). The study of electronic charge density contours shows that change in the bond lengths and bond nature affect the band gap of the compounds. The two non-zero dielectric tensor components and its derivatives show considerable anisotropy between the perpendicular and parallel components. The present work provide accurate information about the combination (hybridization) of orbital, formation of bands and dispersion of non-zero tensor components of $CdGa_2X_4$ (X = S, Se).

Keywords — Electronic structure, optical properties, semiconductors.