Ab- initio study of the electronic and optical properties of the Silver-Copper halides $Ag_{1-x}Cu_xM$(M= Br and Cl)

M. Boukhtouta, H. Meradji and S. Ghemid

Laboratoire LPR, Département de Physique, Faculté des Sciences, Université Badji Mokhtar, Annaba, Algeria.

Abstract

In order to study the electronic and optical properties of the $Ag_{1-x}Cu_xM$ (M= Br and Cl), we performed an ab initio calculations, using the full-potential with the mixed basis (FP-LAPW) plus local orbitals method within the density functional theory (DFT) method. For the band structures as well as total and atom projected densities of states are computed by using the generalized-gradient approximation (WC-GGA) and modified Becke-Johnson (MBJ) of the exchange-correlation energy. The MBJ approximation show a significant amelioration with respect to the experimental data and the values are better than those obtained by the WC-GGA approach. It is worth noting that in contrast to the two compounds AgBr, CuBr and CuCl have direct gap but AgCl has an indirect one (Γ-Δ_{min}). The different interband transitions have been determined from the imaginary part of the dielectric function. The real and imaginary parts of the dielectric function and the reflectivity are calculated. We have presented the assignment of the different optical transitions existing in these compounds from the imaginary part of the dielectric function spectra with respect to their correspondence in the electronic band.

Keywords: Silver and copper halides; ab initio calculation; FP-LAPW; Electronic properties; Optical properties.