Density functional calculation for the first and second harmonic generation of the chalcopyrite Ga_2AsSb

Abstract

An ab initio study of the band structure, density of states, topology of the electron density and the spectral features of the linear and non-linear optical properties of the Ga_2AsSb chalcopyrite are presented. The lattice parameters (a, c), the internal structure parameter, u, describing the position of Ga atom and the (c/a) ratio are optimized. The covalent bonding character is predicted via analyzing the electron density at the equilibrium geometry. The linear optical properties namely the real and imaginary parts of dielectric function, reflectivity, electron energy loss function and refractive index are calculated. This compound has a large uniaxial dielectric anisotropy and a large negative birefringence. Based on the density functional theory the non-linear optical properties are calculated and their spectra are analyzed.