

ABSTRACT

The compound CsSrF₃ phase stability, phase transformation, electronic band structure, and optical characteristics are tailored by Mg-doping computed in CASTEP code. The phase of CsSrF₃ is transformed from cubic to pseudo-cubic tetragonal phase at the doping concentration of 4.22% and 7.04%. The value of band gap (E_g) decreases from 5.677 eV to 2.621 eV. The nature of E_g indirect in case of pure (about R-G symmetry points) and Mg-doping concentration of 1.40%, 4.22% (about R-X symmetry points). The E_g turns into direct at 7.04% Mg doping concentration (Z-Z symmetry point). In optical characteristics, red shift is identified in absorption spectra. The refractive index (n) is increased from 1.43 to 2.01 with Mg-doping.