ABSTRACT

The structural, electronic and optical properties of Rhombohedral pure and strontium doped $MgTiO_3$ perovskite have been investigated by the methodology of all-electron self-consistent ultra-soft pseudopotential plane wave in PBE Generalized Gradient density approximations. The computed optimized structural parameters for pure $MgTiO_3$ are nearly in agreement with the literature values and optimized structural parameters for strontium doped (1.41%, 4.23% and 7.05%) $MgTiO_3$ are presented newly. The electronic band structure of both pure and strontium doped $MgTiO_3$ showed indirect band transition with the bandgap values of 3.596 eV-3.262 eV, respectively. The degree of localized electrons in different bands is confirmed by total and partial densities of states. The transitions in optical properties of pure and strontium doped $MgTiO_3$ material were recognized by assigning corresponding peaks obtained and are discussed in line of structural-electronic determinations. This is the sole theoretical study of rhombohedral crystal structure of strontium doped $MgTiO_3$ as far as we know.