ABSTRACT

The structural, electronic and optical properties of Rhombohedral pure and beryllium doped $NaCaF_3$ perovskite have been investigated by the methodology of all-electron self-consistent ultra-soft pseudo potential plane wave in PBE Generalized Gradient density approximations. The computed optimized structural parameters for pure $NaCaF_3$ are nearly in agreement with the literature values and optimized structural parameters for Beryllium doped (1.41 %, 2.82 %, 4.23 % and 7.05%) $NaCaF_3$ are presented recently. The electronic band structure of both pure and beryllium doped $NaCaF_3$ showed indirect band transition with the band gap values of 4.741eV 0.640 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 Beryllium doped $NaCaF_3$ 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 beryllium doped $NaCaF_3$ as far as we know.