ABSTRACT

All-electron self-consistent ultra-soft pseudo potential plane wave method within PBE Generalized Gradient density approximations are used to investigate structural, electronic and optical properties of cubic pure and magnesium doped $NaCaF_3$ fluoro-perovskite. Our evaluated optimized structural parameters for pure $NaCaF_3$ are well in agreement with the already reported results and optimized structural parameters for magnesium doped (1.41%, 2.82% and 4.23%) $NaCaF_3$ are reported first time. The electronic band structure calculation for pure and magnesium doped $NaCaF_3$ has revealed a direct band transition with the bandgap values of 4.773eV-3.325eV, respectively. Total and partial densities of states confirm the degree of localized electrons in different bands. The optical transitions in pure and magnesium doped $NaCaF_3$ compounds were identified by assigning corresponding peaks obtained from the dispersion relation for the imaginary part of the dielectric function and are discussed in line of structural-electronic determinations. This is the first theoretical study of cubic crystal structure of magnesium doped $NaCaF_3$ as far as we know.